



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 07:42 PM UTC

PDB ID : 7X7S / pdb_00007x7s
BMRB ID : 18133
Title : Solution structure of human adenylate kinase 1 (hAK1)
Authors : Zhang, H.
Deposited on : 2022-03-10

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

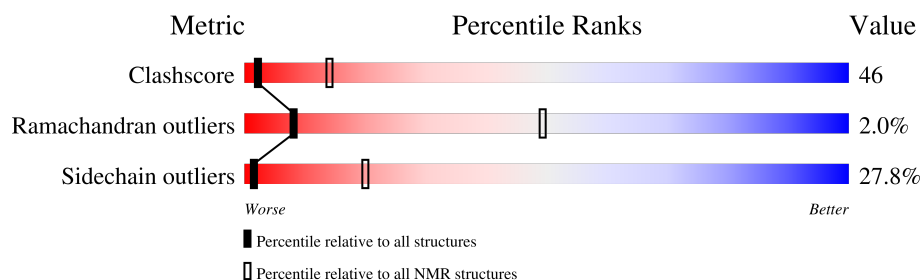
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	199	34% 45% 19% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:199 (194)	0.71	8

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3078 atoms, of which 1561 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	194	Total	C	H	N	O	S	0
			3078	951	1561	264	295	7	

There are 5 discrepancies between the modelled and reference sequences:

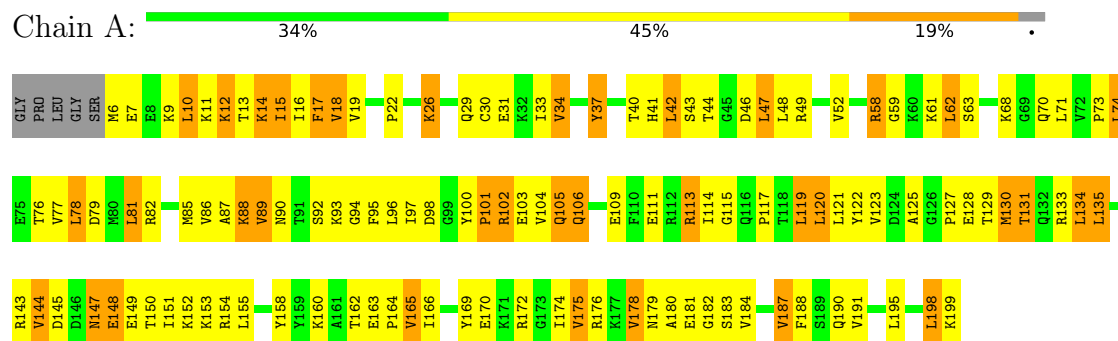
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00568
A	2	PRO	-	expression tag	UNP P00568
A	3	LEU	-	expression tag	UNP P00568
A	4	GLY	-	expression tag	UNP P00568
A	5	SER	-	expression tag	UNP P00568

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: Adenylate kinase isoenzyme 1

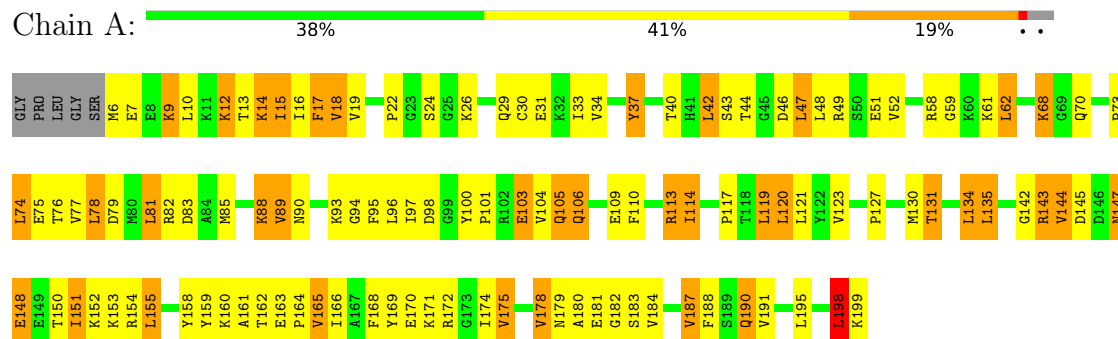


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Adenylate kinase isoenzyme 1



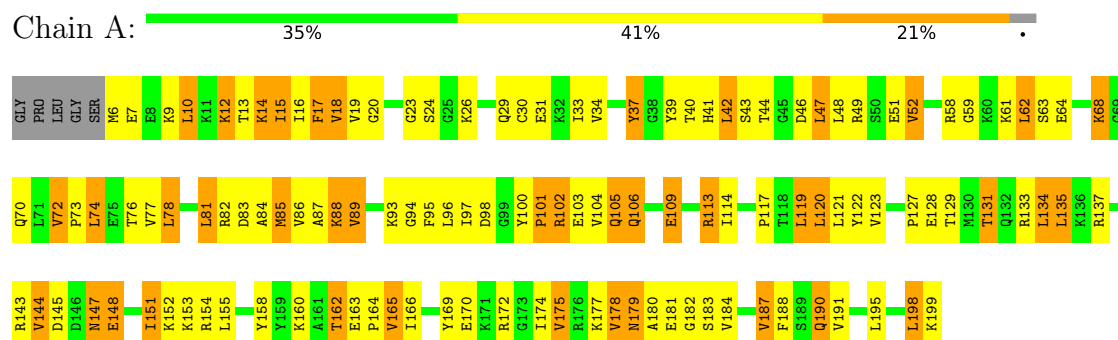
4.2.2 Score per residue for model 2

• Molecule 1: Adenylate kinase isoenzyme 1



4.2.3 Score per residue for model 3

• Molecule 1: Adenylate kinase isoenzyme 1



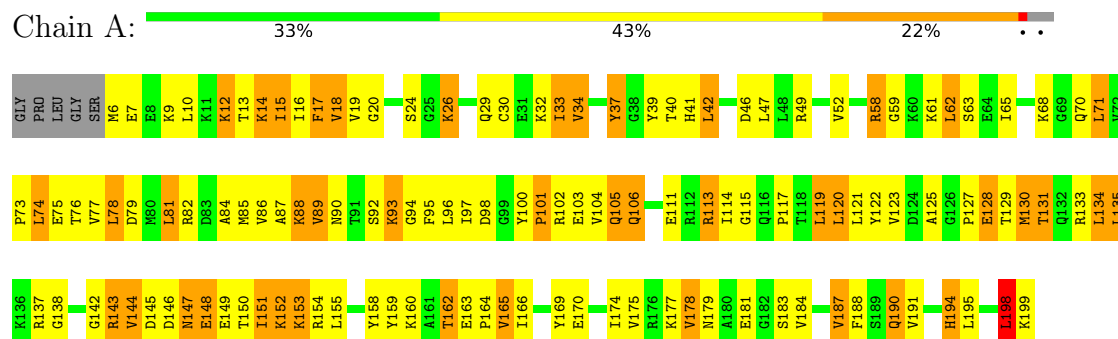
4.2.4 Score per residue for model 4

• Molecule 1: Adenylate kinase isoenzyme 1



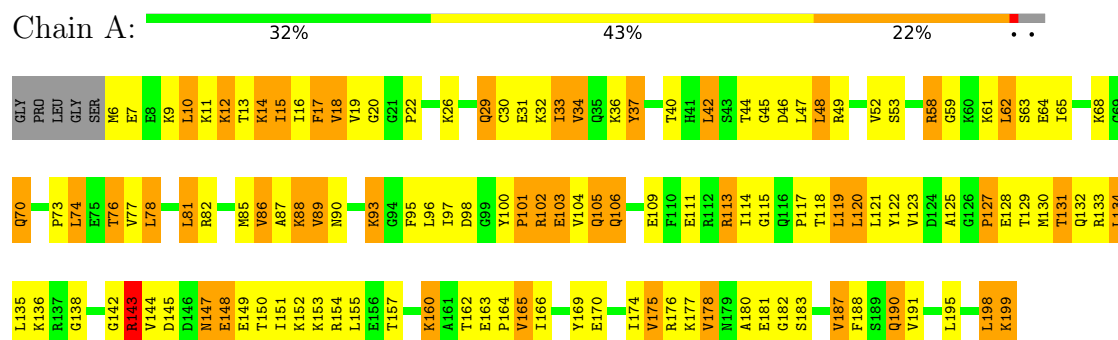
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Adenylate kinase isoenzyme 1



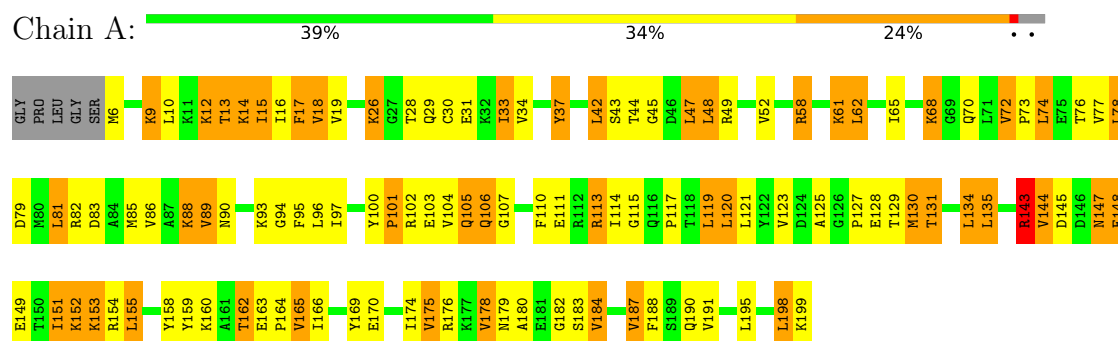
4.2.9 Score per residue for model 9

- Molecule 1: Adenylate kinase isoenzyme 1



4.2.10 Score per residue for model 10

- Molecule 1: Adenylate kinase isoenzyme 1



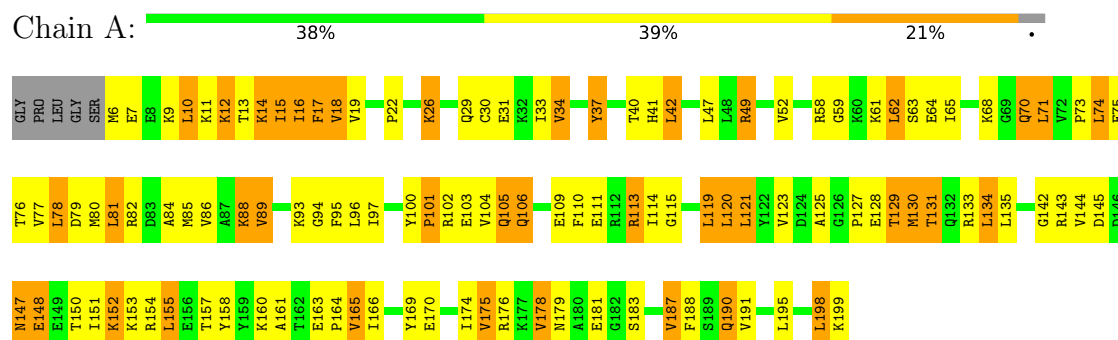
4.2.11 Score per residue for model 11

- Molecule 1: Adenylate kinase isoenzyme 1



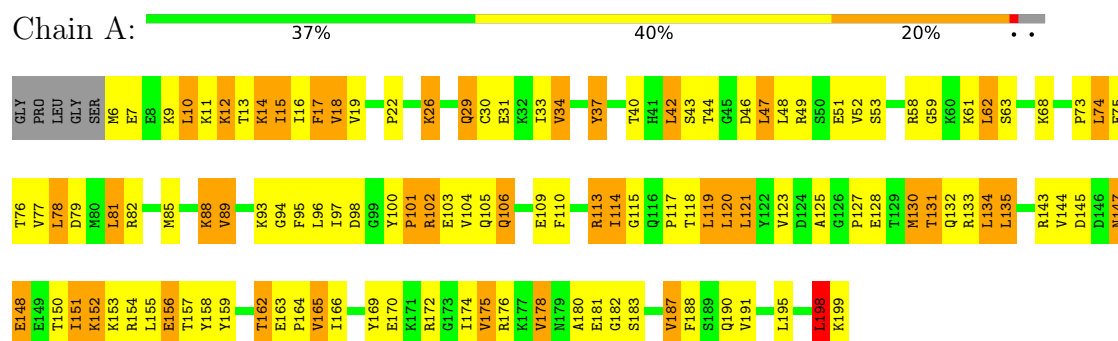
4.2.12 Score per residue for model 12

- Molecule 1: Adenylate kinase isoenzyme 1



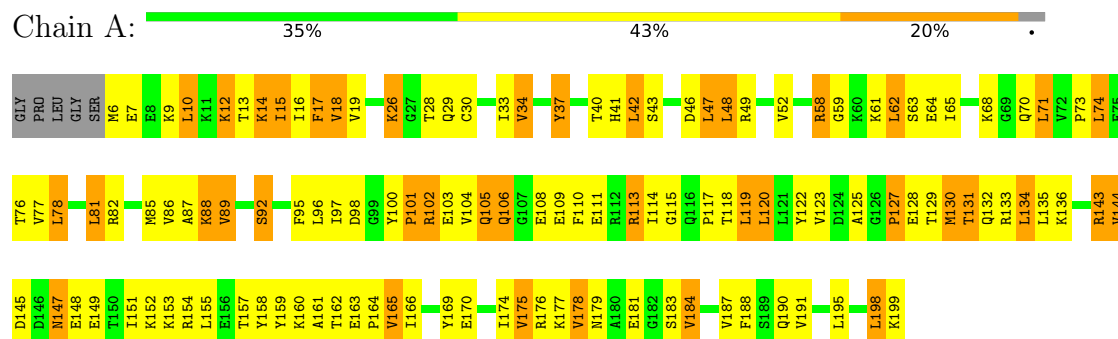
4.2.13 Score per residue for model 13

- Molecule 1: Adenylate kinase isoenzyme 1



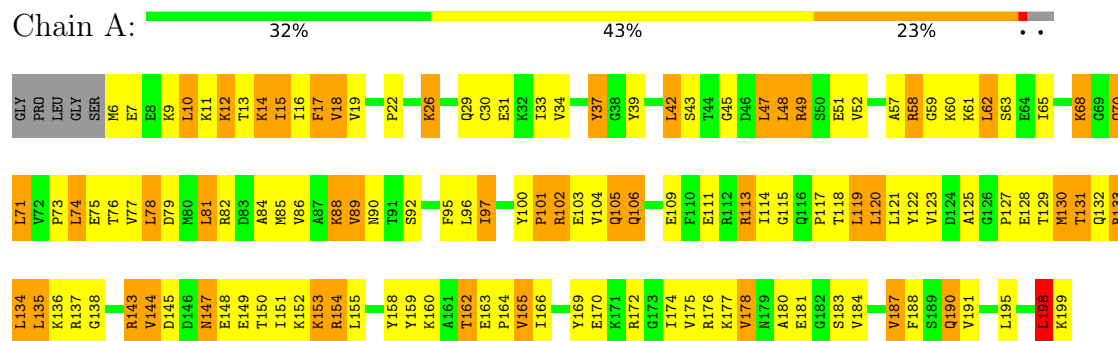
4.2.14 Score per residue for model 14

- Molecule 1: Adenylate kinase isoenzyme 1



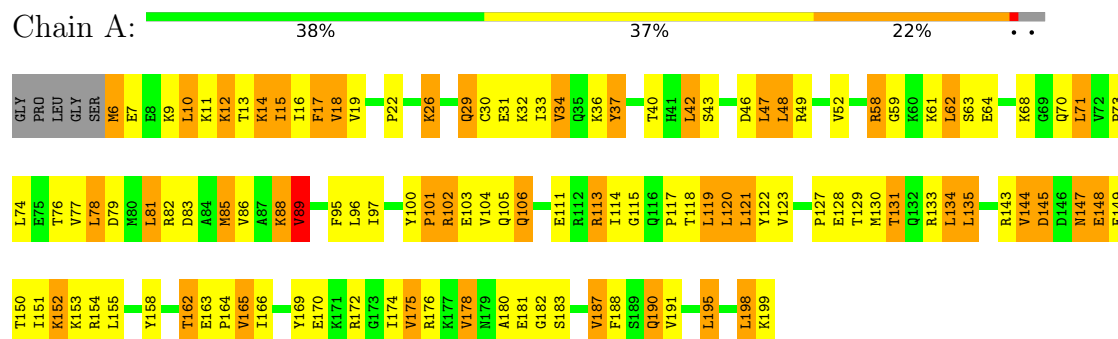
4.2.15 Score per residue for model 15

- Molecule 1: Adenylate kinase isoenzyme 1



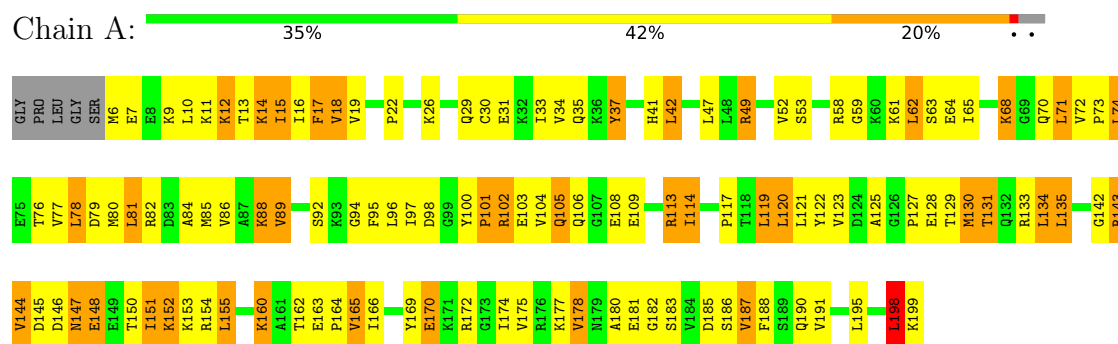
4.2.16 Score per residue for model 16

- Molecule 1: Adenylate kinase isoenzyme 1



4.2.17 Score per residue for model 17

- Molecule 1: Adenylate kinase isoenzyme 1



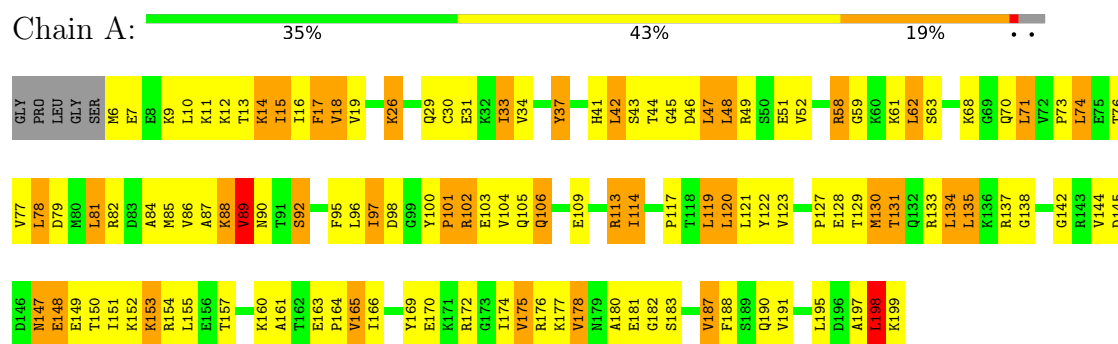
4.2.18 Score per residue for model 18

- Molecule 1: Adenylate kinase isoenzyme 1



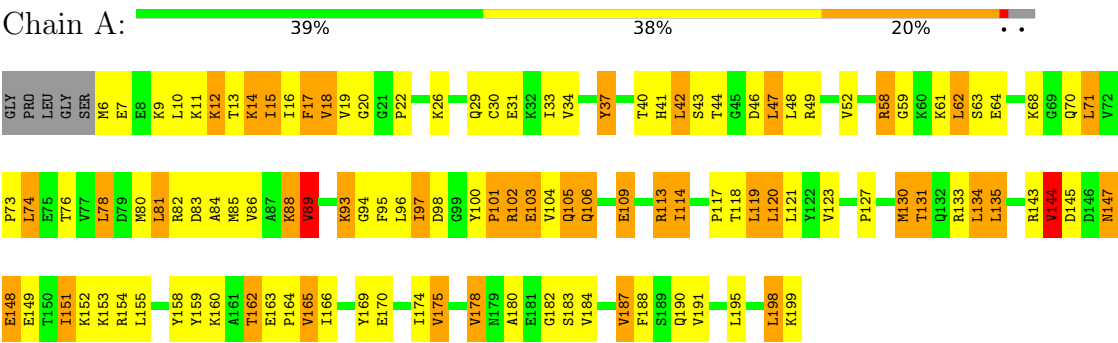
4.2.19 Score per residue for model 19

- Molecule 1: Adenylate kinase isoenzyme 1



4.2.20 Score per residue for model 20

● Molecule 1: Adenylate kinase isoenzyme 1



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
ARIA2alpha	structure calculation	

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	2300
Number of shifts mapped to atoms	2300
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	0.43±0.01	0±0/1536 (0.0± 0.0%)	0.77±0.01	0±0/2058 (0.0± 0.0%)
All	All	0.43	0/30720 (0.0%)	0.77	5/41160 (0.0%)

There are no bond-length outliers.

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	16	ILE	CB-CA-C	-5.44	105.05	111.09	7	2
1	A	44	THR	N-CA-C	-5.24	106.39	112.89	2	2
1	A	170	GLU	N-CA-C	-5.02	106.67	112.89	17	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1517	1561	1558	142±9
All	All	30340	31220	31160	2836

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD21	1:A:84:ALA:HB2	0.89	1.45	2	3
1:A:74:LEU:H	1:A:74:LEU:HD12	0.86	1.27	19	5
1:A:131:THR:OG1	1:A:151:ILE:HG21	0.83	1.73	3	19
1:A:74:LEU:HD12	1:A:74:LEU:N	0.82	1.88	5	17
1:A:198:LEU:HD13	1:A:199:LYS:N	0.81	1.90	7	17
1:A:198:LEU:HD23	1:A:199:LYS:N	0.78	1.92	15	3
1:A:26:LYS:HB3	1:A:123:VAL:HG21	0.78	1.53	12	16
1:A:14:LYS:HB3	1:A:14:LYS:HZ2	0.75	1.41	8	7
1:A:195:LEU:O	1:A:198:LEU:HD22	0.74	1.82	6	3
1:A:15:ILE:HD13	1:A:16:ILE:N	0.74	1.97	13	20
1:A:26:LYS:HB2	1:A:123:VAL:HG21	0.74	1.58	5	1
1:A:74:LEU:HD21	1:A:105:GLN:O	0.73	1.82	7	2
1:A:106:GLN:HE21	1:A:106:GLN:N	0.73	1.82	16	1
1:A:43:SER:O	1:A:47:LEU:HB2	0.73	1.83	20	3
1:A:74:LEU:HD12	1:A:74:LEU:H	0.72	1.42	20	13
1:A:85:MET:HG3	1:A:114:ILE:HG23	0.72	1.60	17	5
1:A:123:VAL:HA	1:A:178:VAL:HG22	0.72	1.60	18	20
1:A:170:GLU:HG2	1:A:175:VAL:HG11	0.71	1.63	19	20
1:A:190:GLN:CD	1:A:191:VAL:N	0.71	2.49	18	1
1:A:82:ARG:O	1:A:86:VAL:HG13	0.70	1.86	10	10
1:A:135:LEU:HD23	1:A:151:ILE:HG12	0.70	1.63	14	1
1:A:19:VAL:HG22	1:A:120:LEU:HD21	0.70	1.62	19	1
1:A:114:ILE:HD13	1:A:114:ILE:N	0.70	2.01	19	6
1:A:147:ASN:O	1:A:151:ILE:HD13	0.70	1.87	3	19
1:A:26:LYS:HZ1	1:A:99:GLY:HA2	0.70	1.46	18	1
1:A:74:LEU:HD13	1:A:105:GLN:O	0.69	1.87	11	2
1:A:42:LEU:O	1:A:97:ILE:HA	0.69	1.87	3	20
1:A:72:VAL:HG13	1:A:77:VAL:HG21	0.69	1.65	10	3
1:A:71:LEU:H	1:A:71:LEU:HD22	0.68	1.48	19	10
1:A:198:LEU:HD13	1:A:199:LYS:H	0.68	1.48	16	14
1:A:58:ARG:HG3	1:A:59:GLY:N	0.68	2.02	7	5
1:A:18:VAL:HG21	1:A:30:CYS:SG	0.68	2.29	15	10
1:A:15:ILE:HD13	1:A:16:ILE:H	0.68	1.48	20	19
1:A:74:LEU:N	1:A:74:LEU:CD1	0.67	2.56	5	15
1:A:123:VAL:HG13	1:A:180:ALA:HB3	0.67	1.65	2	12
1:A:74:LEU:HD23	1:A:105:GLN:O	0.67	1.90	15	12
1:A:166:ILE:HG23	1:A:175:VAL:HG21	0.67	1.66	8	20
1:A:61:LYS:HG3	1:A:62:LEU:N	0.67	2.04	17	11
1:A:88:LYS:N	1:A:88:LYS:HD3	0.67	2.04	16	4
1:A:119:LEU:HD21	1:A:194:HIS:CE1	0.66	2.26	8	1
1:A:87:ALA:HB3	1:A:88:LYS:HZ2	0.66	1.50	19	3
1:A:144:VAL:HG23	1:A:145:ASP:H	0.65	1.51	14	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLY:N	1:A:26:LYS:HZ1	0.65	1.90	3	5
1:A:31:GLU:O	1:A:34:VAL:HG22	0.64	1.91	5	15
1:A:87:ALA:HB3	1:A:88:LYS:HZ3	0.64	1.53	18	3
1:A:13:THR:HG21	1:A:95:PHE:HE1	0.64	1.52	12	16
1:A:42:LEU:HD11	1:A:88:LYS:HZ1	0.63	1.53	16	6
1:A:52:VAL:HG22	1:A:59:GLY:HA2	0.63	1.69	3	1
1:A:58:ARG:HB2	1:A:62:LEU:HD11	0.63	1.69	18	5
1:A:178:VAL:HB	1:A:190:GLN:CD	0.63	2.18	18	1
1:A:29:GLN:HE21	1:A:187:VAL:HG13	0.63	1.54	12	10
1:A:144:VAL:HG13	1:A:145:ASP:H	0.63	1.54	16	1
1:A:148:GLU:O	1:A:151:ILE:HB	0.63	1.93	13	20
1:A:135:LEU:HD23	1:A:151:ILE:HD11	0.62	1.71	3	9
1:A:73:PRO:O	1:A:77:VAL:HG12	0.62	1.94	5	1
1:A:103:GLU:H	1:A:106:GLN:NE2	0.62	1.91	11	2
1:A:18:VAL:HG13	1:A:97:ILE:O	0.62	1.95	14	17
1:A:73:PRO:O	1:A:77:VAL:HG23	0.61	1.94	11	18
1:A:88:LYS:HZ2	1:A:88:LYS:H	0.61	1.34	17	3
1:A:39:TYR:OH	1:A:198:LEU:HD21	0.61	1.95	6	2
1:A:41:HIS:O	1:A:42:LEU:HD13	0.61	1.96	12	1
1:A:195:LEU:O	1:A:198:LEU:HD12	0.61	1.95	7	17
1:A:34:VAL:HG12	1:A:96:LEU:HD22	0.61	1.73	5	15
1:A:65:ILE:HG23	1:A:70:GLN:HB2	0.61	1.71	2	7
1:A:58:ARG:O	1:A:62:LEU:HD22	0.60	1.95	4	1
1:A:42:LEU:HD22	1:A:95:PHE:HB3	0.60	1.72	15	19
1:A:48:LEU:HD21	1:A:77:VAL:HG22	0.60	1.73	19	3
1:A:74:LEU:HD23	1:A:78:LEU:HD11	0.60	1.72	7	1
1:A:88:LYS:HZ2	1:A:88:LYS:N	0.60	1.95	12	1
1:A:81:LEU:HD21	1:A:97:ILE:HD13	0.60	1.74	17	13
1:A:6:MET:HA	1:A:89:VAL:HG21	0.60	1.71	17	5
1:A:48:LEU:CD1	1:A:48:LEU:N	0.60	2.65	19	4
1:A:128:GLU:HG2	1:A:129:THR:N	0.60	2.11	12	2
1:A:144:VAL:HG11	1:A:154:ARG:HE	0.60	1.55	16	1
1:A:33:ILE:HG23	1:A:195:LEU:HD13	0.60	1.73	18	16
1:A:183:SER:O	1:A:187:VAL:HG12	0.60	1.97	8	19
1:A:42:LEU:N	1:A:42:LEU:HD22	0.60	2.11	12	1
1:A:78:LEU:N	1:A:78:LEU:HD23	0.60	2.12	7	12
1:A:151:ILE:HA	1:A:154:ARG:HH12	0.60	1.57	14	7
1:A:61:LYS:HG3	1:A:62:LEU:HG	0.60	1.74	6	7
1:A:78:LEU:HD12	1:A:109:GLU:HB3	0.59	1.74	20	12
1:A:135:LEU:O	1:A:135:LEU:HD22	0.59	1.97	11	16
1:A:47:LEU:HD11	1:A:81:LEU:HD13	0.59	1.73	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:HA	1:A:97:ILE:HB	0.59	1.73	19	18
1:A:120:LEU:O	1:A:120:LEU:HD13	0.59	1.97	19	1
1:A:47:LEU:HD11	1:A:81:LEU:N	0.59	2.12	20	1
1:A:9:LYS:HG3	1:A:89:VAL:HB	0.59	1.74	18	14
1:A:117:PRO:HB2	1:A:172:ARG:HD3	0.59	1.74	2	1
1:A:49:ARG:O	1:A:52:VAL:HG22	0.59	1.98	4	15
1:A:68:LYS:HB2	1:A:70:GLN:HG3	0.59	1.75	3	9
1:A:16:ILE:HG12	1:A:119:LEU:HB3	0.59	1.75	15	20
1:A:29:GLN:HE21	1:A:187:VAL:HB	0.58	1.58	14	1
1:A:119:LEU:HD22	1:A:174:ILE:O	0.58	1.97	2	20
1:A:48:LEU:O	1:A:51:GLU:HG2	0.58	1.98	15	1
1:A:74:LEU:O	1:A:78:LEU:HD12	0.58	1.98	16	1
1:A:10:LEU:HA	1:A:13:THR:HB	0.58	1.74	7	18
1:A:47:LEU:HD21	1:A:84:ALA:HB3	0.58	1.74	12	2
1:A:78:LEU:HD12	1:A:113:ARG:NH1	0.58	2.13	11	3
1:A:41:HIS:C	1:A:42:LEU:HD13	0.58	2.24	12	1
1:A:82:ARG:HB2	1:A:113:ARG:HB2	0.58	1.74	20	7
1:A:14:LYS:HB3	1:A:14:LYS:NZ	0.58	2.14	7	6
1:A:143:ARG:HD2	1:A:144:VAL:HG22	0.58	1.74	11	6
1:A:33:ILE:O	1:A:37:TYR:HB2	0.58	1.99	16	20
1:A:114:ILE:N	1:A:114:ILE:CD1	0.58	2.67	18	7
1:A:20:GLY:N	1:A:26:LYS:HZ2	0.58	1.97	11	1
1:A:78:LEU:HB2	1:A:113:ARG:NH1	0.57	2.14	15	7
1:A:79:ASP:HB2	1:A:113:ARG:NH2	0.57	2.14	15	13
1:A:119:LEU:HD13	1:A:120:LEU:N	0.57	2.14	11	20
1:A:89:VAL:HG13	1:A:95:PHE:CZ	0.57	2.34	5	9
1:A:103:GLU:HG2	1:A:106:GLN:NE2	0.57	2.13	15	7
1:A:71:LEU:H	1:A:71:LEU:HD13	0.57	1.60	4	3
1:A:143:ARG:NE	1:A:143:ARG:HA	0.57	2.14	7	7
1:A:51:GLU:OE2	1:A:62:LEU:HD13	0.57	1.98	15	1
1:A:16:ILE:HA	1:A:119:LEU:O	0.57	2.00	9	20
1:A:117:PRO:O	1:A:174:ILE:HG21	0.57	2.00	6	19
1:A:114:ILE:HD12	1:A:114:ILE:N	0.57	2.14	10	14
1:A:42:LEU:HD11	1:A:88:LYS:NZ	0.57	2.15	13	10
1:A:78:LEU:HD13	1:A:110:PHE:N	0.56	2.14	14	9
1:A:6:MET:HG2	1:A:85:MET:SD	0.56	2.39	20	3
1:A:15:ILE:H	1:A:118:THR:HB	0.56	1.58	13	9
1:A:147:ASN:O	1:A:147:ASN:ND2	0.56	2.39	13	7
1:A:147:ASN:HD22	1:A:147:ASN:N	0.56	1.98	1	5
1:A:48:LEU:HD21	1:A:77:VAL:HA	0.56	1.78	9	5
1:A:78:LEU:HD11	1:A:106:GLN:O	0.56	2.01	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:TYR:CD1	1:A:37:TYR:N	0.56	2.72	6	20
1:A:81:LEU:O	1:A:85:MET:HG2	0.56	2.00	12	5
1:A:103:GLU:H	1:A:106:GLN:HE21	0.56	1.44	17	2
1:A:125:ALA:HB1	1:A:130:MET:HG2	0.56	1.76	13	12
1:A:61:LYS:HG3	1:A:62:LEU:H	0.56	1.60	17	5
1:A:183:SER:O	1:A:187:VAL:HG23	0.56	1.99	14	1
1:A:24:SER:HB2	1:A:123:VAL:HG12	0.56	1.78	3	3
1:A:135:LEU:HA	1:A:143:ARG:HG3	0.56	1.77	13	3
1:A:191:VAL:O	1:A:195:LEU:HG	0.56	2.01	18	20
1:A:29:GLN:HE21	1:A:187:VAL:HG22	0.56	1.60	17	8
1:A:81:LEU:HD12	1:A:85:MET:HG2	0.56	1.78	17	2
1:A:88:LYS:N	1:A:88:LYS:CD	0.56	2.69	16	1
1:A:120:LEU:HD12	1:A:175:VAL:HA	0.56	1.77	19	1
1:A:198:LEU:HD23	1:A:198:LEU:C	0.55	2.26	6	3
1:A:29:GLN:NE2	1:A:187:VAL:HG13	0.55	2.16	16	14
1:A:9:LYS:N	1:A:9:LYS:HD3	0.55	2.16	6	3
1:A:149:GLU:HG2	1:A:153:LYS:HZ1	0.55	1.61	7	3
1:A:121:LEU:HD21	1:A:191:VAL:HG23	0.55	1.76	5	6
1:A:128:GLU:HG3	1:A:129:THR:N	0.55	2.16	16	9
1:A:19:VAL:HG22	1:A:120:LEU:CD1	0.55	2.31	9	19
1:A:152:LYS:HD2	1:A:152:LYS:C	0.55	2.26	9	19
1:A:6:MET:O	1:A:89:VAL:HG11	0.55	2.02	19	8
1:A:33:ILE:CG2	1:A:195:LEU:HD13	0.55	2.32	8	16
1:A:106:GLN:NE2	1:A:106:GLN:N	0.55	2.53	9	16
1:A:82:ARG:HB3	1:A:113:ARG:HB2	0.55	1.77	14	9
1:A:44:THR:O	1:A:48:LEU:HD22	0.55	2.02	7	4
1:A:172:ARG:N	1:A:172:ARG:HD2	0.55	2.17	19	8
1:A:78:LEU:HD22	1:A:100:TYR:OH	0.55	2.02	19	4
1:A:154:ARG:HG2	1:A:154:ARG:HH11	0.55	1.61	1	5
1:A:88:LYS:HD2	1:A:88:LYS:H	0.55	1.61	14	5
1:A:85:MET:O	1:A:88:LYS:NZ	0.55	2.40	1	2
1:A:6:MET:SD	1:A:7:GLU:HG3	0.55	2.42	2	2
1:A:105:GLN:HG2	1:A:106:GLN:NE2	0.55	2.16	15	2
1:A:58:ARG:HG2	1:A:62:LEU:HD11	0.55	1.78	3	9
1:A:14:LYS:HD2	1:A:15:ILE:H	0.54	1.60	7	8
1:A:14:LYS:HE2	1:A:16:ILE:HG12	0.54	1.78	2	12
1:A:169:TYR:HB3	1:A:174:ILE:HD11	0.54	1.80	1	20
1:A:19:VAL:HG22	1:A:120:LEU:HD11	0.54	1.80	1	19
1:A:131:THR:O	1:A:135:LEU:HG	0.54	2.02	14	1
1:A:43:SER:O	1:A:47:LEU:HD13	0.54	2.02	3	9
1:A:48:LEU:HD11	1:A:77:VAL:HG22	0.54	1.77	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ILE:HD12	1:A:154:ARG:NH2	0.54	2.17	13	4
1:A:88:LYS:HD3	1:A:88:LYS:H	0.54	1.62	16	1
1:A:122:TYR:HB3	1:A:177:LYS:HG2	0.54	1.80	11	9
1:A:74:LEU:HB3	1:A:78:LEU:HD11	0.54	1.79	16	2
1:A:6:MET:SD	1:A:7:GLU:N	0.54	2.81	20	15
1:A:14:LYS:NZ	1:A:198:LEU:O	0.54	2.40	2	6
1:A:16:ILE:HG21	1:A:121:LEU:HD12	0.54	1.80	12	2
1:A:147:ASN:C	1:A:147:ASN:ND2	0.54	2.64	18	2
1:A:9:LYS:O	1:A:12:LYS:HG3	0.54	2.03	12	5
1:A:33:ILE:N	1:A:33:ILE:HD13	0.54	2.18	8	5
1:A:134:LEU:HG	1:A:135:LEU:N	0.53	2.18	12	12
1:A:18:VAL:HB	1:A:121:LEU:HB2	0.53	1.81	20	4
1:A:26:LYS:HZ2	1:A:123:VAL:HB	0.53	1.62	5	1
1:A:74:LEU:HD22	1:A:106:GLN:HG3	0.53	1.80	11	2
1:A:104:VAL:HG12	1:A:165:VAL:HA	0.53	1.80	2	13
1:A:18:VAL:HG23	1:A:26:LYS:NZ	0.53	2.18	19	2
1:A:103:GLU:HG2	1:A:106:GLN:HE21	0.53	1.62	3	11
1:A:26:LYS:HG2	1:A:27:GLY:N	0.53	2.17	5	1
1:A:73:PRO:HG2	1:A:76:THR:OG1	0.53	2.04	20	14
1:A:95:PHE:C	1:A:96:LEU:HD12	0.53	2.29	12	3
1:A:160:LYS:HD3	1:A:160:LYS:H	0.53	1.62	18	5
1:A:74:LEU:HG	1:A:105:GLN:HG3	0.53	1.78	15	1
1:A:104:VAL:HG11	1:A:164:PRO:HB2	0.53	1.80	19	16
1:A:187:VAL:O	1:A:191:VAL:HG12	0.53	2.04	14	12
1:A:64:GLU:HB2	1:A:68:LYS:HE2	0.53	1.80	20	3
1:A:29:GLN:O	1:A:33:ILE:HG13	0.53	2.04	20	13
1:A:26:LYS:HB2	1:A:123:VAL:CG2	0.53	2.33	5	1
1:A:14:LYS:O	1:A:94:GLY:HA2	0.53	2.04	17	11
1:A:44:THR:O	1:A:48:LEU:HD12	0.53	2.04	1	5
1:A:29:GLN:HE22	1:A:188:PHE:N	0.52	2.02	13	19
1:A:85:MET:HG2	1:A:114:ILE:HG23	0.52	1.80	20	3
1:A:71:LEU:N	1:A:71:LEU:HD22	0.52	2.19	11	3
1:A:134:LEU:HD21	1:A:143:ARG:HH21	0.52	1.64	13	2
1:A:58:ARG:HG3	1:A:59:GLY:H	0.52	1.64	1	5
1:A:13:THR:HG23	1:A:93:LYS:O	0.52	2.03	18	5
1:A:134:LEU:HD11	1:A:143:ARG:CZ	0.52	2.34	15	2
1:A:130:MET:O	1:A:134:LEU:HB3	0.52	2.05	20	16
1:A:126:GLY:H	1:A:181:GLU:HB3	0.52	1.65	18	1
1:A:15:ILE:HD12	1:A:17:PHE:CD1	0.52	2.40	6	20
1:A:58:ARG:HG2	1:A:62:LEU:HD21	0.52	1.80	4	1
1:A:47:LEU:HD21	1:A:84:ALA:CB	0.52	2.34	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:LYS:HD2	1:A:161:ALA:N	0.52	2.20	14	5
1:A:111:GLU:HA	1:A:115:GLY:O	0.52	2.05	15	12
1:A:158:TYR:O	1:A:162:THR:HB	0.52	2.04	10	10
1:A:93:LYS:HD3	1:A:93:LYS:H	0.52	1.64	12	4
1:A:32:LYS:O	1:A:36:LYS:HG2	0.52	2.05	16	2
1:A:34:VAL:HG12	1:A:96:LEU:CD2	0.51	2.35	2	15
1:A:163:GLU:N	1:A:164:PRO:HD2	0.51	2.20	12	20
1:A:104:VAL:O	1:A:108:GLU:N	0.51	2.43	11	4
1:A:82:ARG:HA	1:A:85:MET:HG3	0.51	1.82	18	2
1:A:9:LYS:O	1:A:12:LYS:HG2	0.51	2.06	2	12
1:A:9:LYS:HB2	1:A:89:VAL:HG12	0.51	1.82	13	7
1:A:135:LEU:HD21	1:A:147:ASN:N	0.51	2.20	3	5
1:A:85:MET:O	1:A:89:VAL:HG22	0.51	2.05	1	5
1:A:144:VAL:HG21	1:A:154:ARG:HH21	0.51	1.66	9	2
1:A:120:LEU:HD13	1:A:120:LEU:C	0.51	2.30	19	1
1:A:15:ILE:HD12	1:A:17:PHE:CE1	0.51	2.40	20	8
1:A:81:LEU:HG	1:A:114:ILE:HG12	0.51	1.81	7	10
1:A:36:LYS:HG3	1:A:37:TYR:CD1	0.51	2.40	16	2
1:A:145:ASP:HB3	1:A:147:ASN:ND2	0.51	2.20	17	10
1:A:102:ARG:N	1:A:102:ARG:CD	0.51	2.73	20	5
1:A:121:LEU:CD2	1:A:191:VAL:HG23	0.51	2.35	8	10
1:A:151:ILE:HA	1:A:154:ARG:NH1	0.51	2.21	5	7
1:A:85:MET:SD	1:A:114:ILE:HG23	0.51	2.46	14	1
1:A:10:LEU:HD23	1:A:115:GLY:HA3	0.51	1.81	15	5
1:A:30:CYS:O	1:A:34:VAL:HG13	0.51	2.06	5	1
1:A:51:GLU:HB2	1:A:58:ARG:HD3	0.51	1.83	15	1
1:A:14:LYS:NZ	1:A:16:ILE:HG13	0.50	2.21	5	2
1:A:120:LEU:HD22	1:A:121:LEU:N	0.50	2.20	19	1
1:A:74:LEU:HD13	1:A:105:GLN:C	0.50	2.31	11	2
1:A:18:VAL:HG22	1:A:98:ASP:HA	0.50	1.81	3	5
1:A:14:LYS:NZ	1:A:119:LEU:HB2	0.50	2.22	4	1
1:A:78:LEU:HD12	1:A:113:ARG:HH11	0.50	1.65	11	5
1:A:121:LEU:HD23	1:A:191:VAL:HG23	0.50	1.82	8	1
1:A:174:ILE:HD12	1:A:175:VAL:N	0.50	2.21	15	15
1:A:149:GLU:HG2	1:A:153:LYS:NZ	0.50	2.22	7	4
1:A:104:VAL:N	1:A:165:VAL:HG22	0.50	2.21	6	16
1:A:166:ILE:O	1:A:170:GLU:HG3	0.50	2.06	12	20
1:A:47:LEU:HD23	1:A:81:LEU:HD22	0.50	1.82	11	4
1:A:51:GLU:HB3	1:A:58:ARG:NE	0.50	2.21	3	4
1:A:179:ASN:HD22	1:A:179:ASN:N	0.50	2.04	3	1
1:A:19:VAL:HG12	1:A:100:TYR:HB3	0.50	1.83	3	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:GLN:N	1:A:106:GLN:HE21	0.50	2.03	9	8
1:A:9:LYS:HD2	1:A:89:VAL:HB	0.49	1.84	12	1
1:A:102:ARG:O	1:A:165:VAL:HG21	0.49	2.08	12	14
1:A:114:ILE:HD12	1:A:114:ILE:H	0.49	1.67	10	12
1:A:6:MET:HB2	1:A:86:VAL:HG12	0.49	1.84	6	4
1:A:190:GLN:H	1:A:190:GLN:HE21	0.49	1.50	9	3
1:A:22:PRO:O	1:A:130:MET:HE2	0.49	2.06	1	2
1:A:48:LEU:N	1:A:48:LEU:CD2	0.49	2.75	5	7
1:A:149:GLU:HG3	1:A:153:LYS:NZ	0.49	2.22	14	6
1:A:43:SER:O	1:A:47:LEU:CB	0.49	2.58	20	1
1:A:101:PRO:HB2	1:A:106:GLN:NE2	0.49	2.22	17	2
1:A:143:ARG:HA	1:A:143:ARG:HE	0.49	1.68	1	2
1:A:100:TYR:CG	1:A:101:PRO:HD2	0.49	2.42	16	19
1:A:138:GLY:HA2	1:A:142:GLY:H	0.49	1.67	8	4
1:A:74:LEU:H	1:A:74:LEU:HD23	0.49	1.68	17	1
1:A:86:VAL:HA	1:A:89:VAL:CG2	0.49	2.38	14	7
1:A:151:ILE:O	1:A:155:LEU:HB2	0.49	2.08	17	3
1:A:58:ARG:HH21	1:A:76:THR:HG22	0.49	1.67	14	3
1:A:180:ALA:C	1:A:182:GLY:H	0.49	2.16	18	7
1:A:34:VAL:HG11	1:A:41:HIS:HB2	0.49	1.84	12	12
1:A:92:SER:HB3	1:A:95:PHE:CZ	0.49	2.43	6	8
1:A:14:LYS:CE	1:A:16:ILE:HG13	0.49	2.38	15	2
1:A:22:PRO:O	1:A:134:LEU:HD22	0.48	2.08	17	11
1:A:7:GLU:O	1:A:11:LYS:HD3	0.48	2.08	19	9
1:A:14:LYS:HD2	1:A:15:ILE:N	0.48	2.23	7	8
1:A:46:ASP:O	1:A:49:ARG:HB3	0.48	2.08	6	7
1:A:49:ARG:O	1:A:49:ARG:HD3	0.48	2.08	18	5
1:A:135:LEU:HD23	1:A:151:ILE:CG1	0.48	2.36	14	1
1:A:51:GLU:HB2	1:A:58:ARG:CD	0.48	2.38	15	1
1:A:74:LEU:HG	1:A:106:GLN:CD	0.48	2.33	1	6
1:A:26:LYS:HB3	1:A:123:VAL:CG2	0.48	2.39	18	12
1:A:85:MET:HG3	1:A:86:VAL:N	0.48	2.24	9	3
1:A:103:GLU:HG3	1:A:105:GLN:HG2	0.48	1.85	3	3
1:A:180:ALA:HB2	1:A:187:VAL:HG21	0.48	1.83	1	6
1:A:45:GLY:O	1:A:49:ARG:HB2	0.48	2.08	19	7
1:A:47:LEU:HD22	1:A:80:MET:C	0.48	2.33	5	3
1:A:109:GLU:O	1:A:112:ARG:HB2	0.48	2.08	7	1
1:A:104:VAL:HG12	1:A:165:VAL:CA	0.48	2.38	2	7
1:A:111:GLU:HG3	1:A:117:PRO:HD3	0.48	1.86	2	1
1:A:74:LEU:O	1:A:78:LEU:HG	0.48	2.08	17	8
1:A:85:MET:O	1:A:95:PHE:CE2	0.48	2.66	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:LEU:HA	1:A:143:ARG:HE	0.48	1.67	15	1
1:A:49:ARG:HD2	1:A:52:VAL:HG12	0.48	1.86	3	1
1:A:114:ILE:H	1:A:114:ILE:HD12	0.48	1.69	3	2
1:A:74:LEU:HB2	1:A:78:LEU:HD11	0.48	1.86	17	1
1:A:153:LYS:O	1:A:157:THR:HG23	0.48	2.09	14	7
1:A:131:THR:O	1:A:135:LEU:HB3	0.48	2.08	17	5
1:A:136:LYS:HA	1:A:136:LYS:HE3	0.48	1.85	11	1
1:A:84:ALA:O	1:A:88:LYS:NZ	0.48	2.47	15	2
1:A:88:LYS:HD2	1:A:88:LYS:N	0.48	2.22	14	5
1:A:74:LEU:HA	1:A:77:VAL:HG13	0.48	1.85	5	1
1:A:150:THR:O	1:A:154:ARG:HB2	0.48	2.09	11	5
1:A:37:TYR:N	1:A:37:TYR:HD1	0.48	2.07	6	9
1:A:81:LEU:HD12	1:A:85:MET:CG	0.47	2.39	12	1
1:A:43:SER:C	1:A:47:LEU:HD22	0.47	2.33	11	7
1:A:19:VAL:O	1:A:122:TYR:HA	0.47	2.09	15	6
1:A:102:ARG:CD	1:A:102:ARG:H	0.47	2.21	20	5
1:A:105:GLN:HG2	1:A:106:GLN:HE21	0.47	1.68	15	1
1:A:87:ALA:CB	1:A:88:LYS:HZ2	0.47	2.22	19	1
1:A:155:LEU:HD22	1:A:158:TYR:OH	0.47	2.09	12	3
1:A:134:LEU:HA	1:A:137:ARG:CD	0.47	2.39	15	2
1:A:143:ARG:NE	1:A:144:VAL:HG22	0.47	2.23	14	1
1:A:74:LEU:HG	1:A:106:GLN:HG3	0.47	1.85	16	1
1:A:85:MET:HE1	1:A:95:PHE:CB	0.47	2.40	12	1
1:A:172:ARG:HD2	1:A:172:ARG:H	0.47	1.70	15	4
1:A:198:LEU:C	1:A:198:LEU:HD22	0.47	2.34	18	17
1:A:49:ARG:HA	1:A:52:VAL:HB	0.47	1.85	3	1
1:A:10:LEU:O	1:A:13:THR:O	0.47	2.33	11	2
1:A:34:VAL:HG23	1:A:35:GLN:HE21	0.47	1.70	2	1
1:A:13:THR:HG21	1:A:95:PHE:CE1	0.47	2.40	12	5
1:A:117:PRO:HB2	1:A:174:ILE:HG12	0.47	1.86	11	3
1:A:105:GLN:HB3	1:A:106:GLN:NE2	0.47	2.24	16	8
1:A:87:ALA:HB3	1:A:88:LYS:NZ	0.47	2.23	14	4
1:A:151:ILE:O	1:A:155:LEU:HG	0.47	2.09	11	3
1:A:6:MET:HB3	1:A:86:VAL:HG11	0.47	1.84	12	1
1:A:30:CYS:HA	1:A:33:ILE:HD12	0.47	1.86	13	2
1:A:81:LEU:HG	1:A:114:ILE:HG13	0.47	1.87	19	3
1:A:133:ARG:O	1:A:137:ARG:HG3	0.47	2.10	15	1
1:A:88:LYS:HB3	1:A:92:SER:HB2	0.47	1.86	19	1
1:A:135:LEU:C	1:A:135:LEU:HD13	0.47	2.34	12	11
1:A:52:VAL:HG12	1:A:62:LEU:HD12	0.47	1.86	6	5
1:A:78:LEU:HB2	1:A:113:ARG:CZ	0.47	2.39	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:GLN:HB3	1:A:106:GLN:HE22	0.47	1.70	8	5
1:A:14:LYS:HB2	1:A:14:LYS:NZ	0.47	2.24	18	1
1:A:190:GLN:CD	1:A:191:VAL:H	0.47	2.18	18	1
1:A:135:LEU:HD11	1:A:148:GLU:N	0.47	2.25	19	1
1:A:89:VAL:HA	1:A:95:PHE:HZ	0.47	1.70	18	7
1:A:77:VAL:O	1:A:81:LEU:HB2	0.47	2.10	12	2
1:A:149:GLU:O	1:A:153:LYS:HE2	0.47	2.10	19	1
1:A:14:LYS:HD3	1:A:15:ILE:N	0.46	2.25	4	3
1:A:6:MET:CG	1:A:86:VAL:HG12	0.46	2.41	20	2
1:A:85:MET:SD	1:A:97:ILE:HD11	0.46	2.50	12	1
1:A:135:LEU:HD12	1:A:136:LYS:N	0.46	2.24	14	1
1:A:19:VAL:HG22	1:A:120:LEU:CD2	0.46	2.37	19	1
1:A:78:LEU:HD22	1:A:110:PHE:HD1	0.46	1.69	1	1
1:A:145:ASP:HB2	1:A:150:THR:HG21	0.46	1.86	16	4
1:A:162:THR:HA	1:A:165:VAL:HG23	0.46	1.87	16	11
1:A:37:TYR:OH	1:A:195:LEU:HD12	0.46	2.11	20	5
1:A:128:GLU:O	1:A:132:GLN:HG3	0.46	2.09	4	5
1:A:144:VAL:HG21	1:A:154:ARG:HE	0.46	1.70	13	1
1:A:82:ARG:CA	1:A:114:ILE:HD12	0.46	2.40	17	4
1:A:75:GLU:O	1:A:79:ASP:HB2	0.46	2.11	11	5
1:A:81:LEU:HD12	1:A:81:LEU:O	0.46	2.10	10	12
1:A:145:ASP:HB3	1:A:147:ASN:HD21	0.46	1.71	10	2
1:A:30:CYS:SG	1:A:98:ASP:HB2	0.46	2.51	4	9
1:A:148:GLU:O	1:A:151:ILE:N	0.46	2.49	2	4
1:A:65:ILE:O	1:A:70:GLN:N	0.46	2.49	4	3
1:A:74:LEU:HD13	1:A:75:GLU:H	0.46	1.70	12	5
1:A:105:GLN:HG2	1:A:106:GLN:HE22	0.46	1.69	7	1
1:A:40:THR:CG2	1:A:88:LYS:HZ3	0.46	2.24	16	1
1:A:29:GLN:NE2	1:A:187:VAL:HG22	0.46	2.26	2	2
1:A:174:ILE:HD12	1:A:174:ILE:C	0.46	2.35	19	10
1:A:109:GLU:HA	1:A:112:ARG:HD3	0.46	1.88	7	1
1:A:14:LYS:HZ3	1:A:94:GLY:HA3	0.46	1.70	13	1
1:A:14:LYS:HA	1:A:118:THR:HG21	0.46	1.87	13	2
1:A:82:ARG:O	1:A:86:VAL:HG22	0.46	2.11	18	2
1:A:103:GLU:HA	1:A:165:VAL:HG21	0.46	1.87	15	2
1:A:151:ILE:HD12	1:A:154:ARG:HH21	0.46	1.71	7	2
1:A:120:LEU:HD12	1:A:121:LEU:N	0.46	2.26	17	8
1:A:105:GLN:HB2	1:A:106:GLN:HE22	0.46	1.70	9	2
1:A:72:VAL:CG1	1:A:77:VAL:HG21	0.46	2.39	10	1
1:A:132:GLN:O	1:A:136:LYS:HB2	0.46	2.11	11	1
1:A:134:LEU:O	1:A:137:ARG:HB2	0.46	2.11	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:H	1:A:74:LEU:CD1	0.46	2.04	19	1
1:A:180:ALA:C	1:A:182:GLY:N	0.45	2.73	10	6
1:A:122:TYR:HB3	1:A:177:LYS:HA	0.45	1.87	8	1
1:A:43:SER:O	1:A:47:LEU:HD22	0.45	2.11	15	1
1:A:68:LYS:HB2	1:A:70:GLN:HG2	0.45	1.88	4	3
1:A:179:ASN:O	1:A:187:VAL:HB	0.45	2.11	10	4
1:A:6:MET:HA	1:A:86:VAL:HB	0.45	1.87	12	1
1:A:40:THR:O	1:A:96:LEU:HB2	0.45	2.11	4	13
1:A:46:ASP:HA	1:A:49:ARG:HB2	0.45	1.88	7	8
1:A:133:ARG:HH12	1:A:182:GLY:HA2	0.45	1.72	11	1
1:A:33:ILE:HG12	1:A:195:LEU:HD13	0.45	1.87	1	1
1:A:102:ARG:CD	1:A:102:ARG:C	0.45	2.90	15	2
1:A:95:PHE:O	1:A:96:LEU:HD12	0.45	2.11	12	2
1:A:52:VAL:HB	1:A:63:SER:HB2	0.45	1.88	14	1
1:A:131:THR:O	1:A:135:LEU:HB2	0.45	2.11	19	1
1:A:179:ASN:HB2	1:A:190:GLN:NE2	0.45	2.26	6	5
1:A:49:ARG:HD2	1:A:52:VAL:HG22	0.45	1.89	7	1
1:A:147:ASN:HD21	1:A:150:THR:CB	0.45	2.24	18	2
1:A:179:ASN:HD22	1:A:190:GLN:HE21	0.45	1.54	8	1
1:A:15:ILE:CD1	1:A:16:ILE:N	0.45	2.78	16	4
1:A:47:LEU:HG	1:A:84:ALA:HB3	0.45	1.89	19	2
1:A:144:VAL:HG13	1:A:145:ASP:N	0.45	2.26	16	1
1:A:64:GLU:HB2	1:A:68:LYS:HE3	0.45	1.89	3	3
1:A:134:LEU:HD12	1:A:143:ARG:NH2	0.45	2.27	3	2
1:A:100:TYR:OH	1:A:107:GLY:HA2	0.45	2.12	10	1
1:A:134:LEU:HD11	1:A:143:ARG:NE	0.45	2.27	11	1
1:A:102:ARG:H	1:A:102:ARG:CD	0.45	2.25	17	1
1:A:59:GLY:O	1:A:63:SER:CB	0.45	2.64	8	12
1:A:131:THR:HG23	1:A:135:LEU:HD21	0.45	1.88	14	1
1:A:179:ASN:O	1:A:187:VAL:HG22	0.45	2.12	14	1
1:A:58:ARG:CG	1:A:62:LEU:HD11	0.45	2.42	2	5
1:A:128:GLU:CG	1:A:129:THR:N	0.45	2.80	5	4
1:A:110:PHE:CD1	1:A:114:ILE:HD13	0.45	2.47	11	1
1:A:57:ALA:O	1:A:60:LYS:HB3	0.45	2.12	15	1
1:A:120:LEU:O	1:A:176:ARG:N	0.45	2.50	14	10
1:A:81:LEU:O	1:A:85:MET:N	0.45	2.50	20	2
1:A:103:GLU:CG	1:A:106:GLN:NE2	0.44	2.81	1	5
1:A:88:LYS:O	1:A:90:ASN:N	0.44	2.50	19	2
1:A:87:ALA:HB3	1:A:88:LYS:CE	0.44	2.43	8	1
1:A:28:THR:HB	1:A:184:VAL:HG21	0.44	1.89	10	2
1:A:74:LEU:HD22	1:A:105:GLN:HB3	0.44	1.88	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLN:HG2	1:A:184:VAL:HG22	0.44	1.89	14	1
1:A:88:LYS:O	1:A:89:VAL:C	0.44	2.61	19	15
1:A:147:ASN:HD22	1:A:147:ASN:H	0.44	1.54	17	5
1:A:29:GLN:NE2	1:A:188:PHE:N	0.44	2.64	3	7
1:A:7:GLU:HA	1:A:10:LEU:HB2	0.44	1.88	12	1
1:A:19:VAL:CG1	1:A:100:TYR:HB3	0.44	2.43	18	1
1:A:14:LYS:HB2	1:A:118:THR:HG21	0.44	1.89	13	2
1:A:144:VAL:HG23	1:A:145:ASP:N	0.44	2.28	13	3
1:A:10:LEU:HD22	1:A:85:MET:HE1	0.44	1.89	14	1
1:A:109:GLU:HB3	1:A:113:ARG:HH11	0.44	1.71	15	3
1:A:6:MET:HE2	1:A:82:ARG:HH12	0.44	1.73	4	1
1:A:113:ARG:CG	1:A:114:ILE:HD12	0.44	2.43	7	7
1:A:62:LEU:HD22	1:A:76:THR:HG21	0.44	1.89	7	2
1:A:48:LEU:HD11	1:A:77:VAL:CG2	0.44	2.43	2	1
1:A:14:LYS:HZ1	1:A:119:LEU:HB2	0.44	1.72	4	1
1:A:104:VAL:O	1:A:105:GLN:C	0.44	2.59	11	2
1:A:134:LEU:HD12	1:A:143:ARG:HD2	0.44	1.89	12	1
1:A:64:GLU:O	1:A:68:LYS:HD2	0.44	2.13	14	2
1:A:102:ARG:CD	1:A:102:ARG:N	0.44	2.80	17	1
1:A:19:VAL:HG23	1:A:122:TYR:CD1	0.44	2.47	11	4
1:A:154:ARG:O	1:A:157:THR:OG1	0.44	2.34	13	1
1:A:72:VAL:HG22	1:A:73:PRO:HD2	0.44	1.87	3	2
1:A:88:LYS:C	1:A:90:ASN:N	0.44	2.75	19	9
1:A:20:GLY:N	1:A:26:LYS:NZ	0.44	2.66	11	1
1:A:187:VAL:HA	1:A:190:GLN:HE21	0.44	1.73	14	1
1:A:47:LEU:CD2	1:A:84:ALA:HB2	0.44	2.32	2	1
1:A:81:LEU:HB3	1:A:114:ILE:HD11	0.44	1.89	2	5
1:A:134:LEU:O	1:A:137:ARG:HB3	0.44	2.12	3	2
1:A:85:MET:C	1:A:87:ALA:N	0.44	2.75	5	5
1:A:132:GLN:O	1:A:136:LYS:HG2	0.44	2.13	9	4
1:A:74:LEU:CD2	1:A:105:GLN:O	0.44	2.65	19	3
1:A:86:VAL:HA	1:A:89:VAL:HG22	0.44	1.89	12	1
1:A:130:MET:SD	1:A:134:LEU:HD23	0.44	2.53	20	2
1:A:42:LEU:CD1	1:A:88:LYS:HZ1	0.44	2.24	16	1
1:A:80:MET:O	1:A:84:ALA:N	0.44	2.50	20	1
1:A:147:ASN:ND2	1:A:150:THR:HB	0.44	2.28	1	3
1:A:52:VAL:CG2	1:A:59:GLY:HA2	0.44	2.40	3	1
1:A:59:GLY:O	1:A:63:SER:HB3	0.44	2.13	17	4
1:A:64:GLU:O	1:A:68:LYS:HD3	0.44	2.13	12	2
1:A:93:LYS:N	1:A:93:LYS:HD3	0.44	2.28	13	1
1:A:85:MET:HA	1:A:88:LYS:HE3	0.44	1.89	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ARG:HA	1:A:114:ILE:HD12	0.44	1.90	20	1
1:A:158:TYR:O	1:A:159:TYR:C	0.43	2.61	6	7
1:A:195:LEU:HA	1:A:198:LEU:HD13	0.43	1.88	6	2
1:A:127:PRO:HB3	1:A:155:LEU:HD21	0.43	1.88	9	2
1:A:101:PRO:CB	1:A:106:GLN:HG2	0.43	2.43	15	1
1:A:134:LEU:HD12	1:A:143:ARG:NE	0.43	2.28	20	1
1:A:100:TYR:CD1	1:A:101:PRO:HD2	0.43	2.49	13	3
1:A:133:ARG:NH1	1:A:182:GLY:HA2	0.43	2.28	16	2
1:A:14:LYS:NZ	1:A:198:LEU:HG	0.43	2.27	19	1
1:A:17:PHE:O	1:A:120:LEU:HD23	0.43	2.13	19	1
1:A:93:LYS:HD2	1:A:94:GLY:N	0.43	2.28	6	1
1:A:29:GLN:O	1:A:33:ILE:HG12	0.43	2.13	8	4
1:A:168:PHE:O	1:A:171:LYS:HB3	0.43	2.13	1	1
1:A:180:ALA:HA	1:A:187:VAL:HB	0.43	1.89	20	3
1:A:7:GLU:HG2	1:A:11:LYS:CE	0.43	2.44	12	1
1:A:144:VAL:HG11	1:A:154:ARG:NE	0.43	2.27	16	1
1:A:14:LYS:HZ2	1:A:14:LYS:C	0.43	2.20	1	2
1:A:31:GLU:HB3	1:A:35:GLN:HE21	0.43	1.74	11	1
1:A:85:MET:HA	1:A:88:LYS:NZ	0.43	2.28	15	1
1:A:42:LEU:HB3	1:A:47:LEU:HD21	0.43	1.91	16	1
1:A:7:GLU:HB3	1:A:11:LYS:HE3	0.43	1.89	2	1
1:A:148:GLU:O	1:A:149:GLU:C	0.43	2.62	15	5
1:A:14:LYS:HZ2	1:A:14:LYS:HB3	0.43	1.73	1	1
1:A:147:ASN:HD21	1:A:150:THR:HB	0.43	1.74	18	3
1:A:68:LYS:N	1:A:68:LYS:HD2	0.43	2.29	12	1
1:A:33:ILE:HG12	1:A:195:LEU:CD1	0.43	2.43	1	1
1:A:29:GLN:HE22	1:A:188:PHE:CA	0.43	2.27	15	3
1:A:135:LEU:HD21	1:A:146:ASP:C	0.43	2.39	17	3
1:A:26:LYS:O	1:A:30:CYS:N	0.43	2.52	13	1
1:A:14:LYS:HD3	1:A:15:ILE:H	0.43	1.74	18	1
1:A:51:GLU:HB3	1:A:58:ARG:CD	0.43	2.44	1	3
1:A:82:ARG:HG3	1:A:83:ASP:N	0.43	2.28	10	3
1:A:187:VAL:HA	1:A:190:GLN:NE2	0.43	2.28	16	2
1:A:79:ASP:HB2	1:A:113:ARG:HH21	0.43	1.73	15	1
1:A:143:ARG:NH2	1:A:154:ARG:NH2	0.42	2.67	3	1
1:A:197:ALA:C	1:A:199:LYS:N	0.42	2.76	18	3
1:A:130:MET:HB3	1:A:133:ARG:HH21	0.42	1.74	13	1
1:A:185:ASP:CG	1:A:186:SER:N	0.42	2.77	17	1
1:A:26:LYS:C	1:A:28:THR:N	0.42	2.77	18	1
1:A:158:TYR:C	1:A:158:TYR:CD1	0.42	2.96	11	1
1:A:9:LYS:HD2	1:A:90:ASN:HA	0.42	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:ALA:O	1:A:88:LYS:HE2	0.42	2.14	5	1
1:A:198:LEU:HD13	1:A:198:LEU:C	0.42	2.38	13	2
1:A:103:GLU:CG	1:A:106:GLN:HE21	0.42	2.28	20	3
1:A:29:GLN:NE2	1:A:184:VAL:O	0.42	2.52	11	4
1:A:85:MET:O	1:A:87:ALA:N	0.42	2.53	8	2
1:A:16:ILE:CG2	1:A:121:LEU:HD12	0.42	2.43	12	1
1:A:184:VAL:HA	1:A:187:VAL:CG1	0.42	2.44	1	3
1:A:24:SER:OG	1:A:26:LYS:NZ	0.42	2.52	5	1
1:A:14:LYS:HE2	1:A:119:LEU:HB2	0.42	1.91	6	1
1:A:147:ASN:HD22	1:A:150:THR:H	0.42	1.57	8	1
1:A:71:LEU:H	1:A:71:LEU:CD2	0.42	2.23	20	3
1:A:47:LEU:HD22	1:A:80:MET:CB	0.42	2.44	2	1
1:A:7:GLU:O	1:A:10:LEU:N	0.42	2.53	9	3
1:A:103:GLU:HG3	1:A:105:GLN:HG3	0.42	1.92	9	1
1:A:105:GLN:HB2	1:A:106:GLN:NE2	0.42	2.29	9	2
1:A:149:GLU:HG3	1:A:153:LYS:HZ1	0.42	1.73	10	1
1:A:49:ARG:HD3	1:A:49:ARG:C	0.42	2.39	12	1
1:A:78:LEU:CD1	1:A:109:GLU:HB3	0.42	2.45	17	1
1:A:20:GLY:CA	1:A:26:LYS:HE2	0.42	2.44	2	1
1:A:29:GLN:OE1	1:A:184:VAL:HB	0.42	2.15	8	3
1:A:14:LYS:HZ3	1:A:14:LYS:HB2	0.42	1.75	4	1
1:A:122:TYR:CB	1:A:177:LYS:HA	0.42	2.44	8	1
1:A:65:ILE:HG12	1:A:70:GLN:HB2	0.42	1.90	9	1
1:A:42:LEU:CD2	1:A:95:PHE:HB3	0.42	2.45	12	1
1:A:17:PHE:CZ	1:A:117:PRO:HA	0.42	2.49	10	4
1:A:110:PHE:CE2	1:A:114:ILE:HB	0.42	2.50	10	2
1:A:14:LYS:NZ	1:A:14:LYS:CB	0.42	2.83	7	1
1:A:144:VAL:HG21	1:A:154:ARG:NH2	0.42	2.29	7	1
1:A:83:ASP:O	1:A:86:VAL:HG22	0.42	2.14	10	1
1:A:184:VAL:O	1:A:188:PHE:HB2	0.42	2.15	11	1
1:A:20:GLY:HA3	1:A:26:LYS:HD3	0.42	1.91	18	1
1:A:102:ARG:HE	1:A:158:TYR:HB3	0.41	1.75	4	2
1:A:44:THR:O	1:A:48:LEU:HD23	0.41	2.15	5	1
1:A:165:VAL:HG12	1:A:169:TYR:CE1	0.41	2.50	5	2
1:A:175:VAL:O	1:A:176:ARG:HD2	0.41	2.15	12	3
1:A:197:ALA:O	1:A:199:LYS:N	0.41	2.54	19	1
1:A:135:LEU:CD2	1:A:151:ILE:HD11	0.41	2.45	3	1
1:A:61:LYS:O	1:A:65:ILE:HG12	0.41	2.14	17	2
1:A:190:GLN:NE2	1:A:191:VAL:N	0.41	2.68	18	1
1:A:123:VAL:HG13	1:A:180:ALA:CB	0.41	2.44	1	1
1:A:74:LEU:HD13	1:A:75:GLU:N	0.41	2.31	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:C	1:A:26:LYS:HZ1	0.41	2.22	7	1
1:A:144:VAL:HG21	1:A:154:ARG:NE	0.41	2.30	7	1
1:A:40:THR:HG21	1:A:88:LYS:HE3	0.41	1.92	3	2
1:A:23:GLY:HA3	1:A:134:LEU:HB2	0.41	1.93	5	1
1:A:6:MET:HG3	1:A:86:VAL:HB	0.41	1.90	12	1
1:A:143:ARG:HH22	1:A:154:ARG:NH2	0.41	2.14	15	1
1:A:194:HIS:O	1:A:198:LEU:N	0.41	2.53	8	1
1:A:136:LYS:C	1:A:138:GLY:N	0.41	2.77	15	1
1:A:160:LYS:HD2	1:A:160:LYS:C	0.41	2.41	1	1
1:A:82:ARG:O	1:A:85:MET:HG3	0.41	2.15	10	1
1:A:86:VAL:O	1:A:89:VAL:HG22	0.41	2.16	12	1
1:A:179:ASN:HB2	1:A:190:GLN:HE22	0.41	1.75	14	1
1:A:155:LEU:O	1:A:159:TYR:HB2	0.41	2.14	1	2
1:A:6:MET:N	1:A:9:LYS:HZ3	0.41	2.14	5	1
1:A:155:LEU:HD12	1:A:158:TYR:OH	0.41	2.16	14	1
1:A:23:GLY:HA2	1:A:134:LEU:HD23	0.41	1.92	3	1
1:A:143:ARG:HH21	1:A:154:ARG:NH2	0.41	2.14	4	1
1:A:24:SER:N	1:A:130:MET:SD	0.41	2.94	5	1
1:A:39:TYR:HB3	1:A:96:LEU:HD13	0.41	1.91	6	3
1:A:52:VAL:HB	1:A:59:GLY:HA2	0.41	1.92	7	1
1:A:95:PHE:CD1	1:A:95:PHE:N	0.41	2.88	10	1
1:A:120:LEU:HD23	1:A:175:VAL:HB	0.41	1.91	10	1
1:A:129:THR:OG1	1:A:130:MET:N	0.41	2.54	12	1
1:A:151:ILE:HA	1:A:154:ARG:NH2	0.41	2.31	12	1
1:A:152:LYS:O	1:A:156:GLU:HG2	0.41	2.15	13	1
1:A:154:ARG:CB	1:A:154:ARG:HH11	0.41	2.28	14	1
1:A:48:LEU:HD11	1:A:77:VAL:HA	0.41	1.92	19	2
1:A:49:ARG:O	1:A:49:ARG:HD2	0.41	2.16	16	1
1:A:26:LYS:O	1:A:27:GLY:C	0.41	2.64	18	1
1:A:103:GLU:N	1:A:106:GLN:NE2	0.41	2.66	11	1
1:A:14:LYS:CB	1:A:118:THR:HG21	0.41	2.46	13	1
1:A:88:LYS:HB3	1:A:92:SER:CB	0.41	2.45	19	1
1:A:39:TYR:OH	1:A:198:LEU:HD11	0.40	2.16	3	1
1:A:74:LEU:HB3	1:A:106:GLN:HA	0.40	1.92	4	2
1:A:26:LYS:NZ	1:A:26:LYS:HB3	0.40	2.31	5	1
1:A:195:LEU:HA	1:A:198:LEU:HB3	0.40	1.93	6	1
1:A:105:GLN:NE2	1:A:105:GLN:HA	0.40	2.31	12	2
1:A:46:ASP:HA	1:A:49:ARG:CB	0.40	2.45	9	1
1:A:154:ARG:NH1	1:A:154:ARG:CB	0.40	2.84	14	1
1:A:134:LEU:HD12	1:A:143:ARG:CZ	0.40	2.47	8	1
1:A:160:LYS:O	1:A:164:PRO:HD2	0.40	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ARG:HA	1:A:61:LYS:NZ	0.40	2.31	20	1
1:A:47:LEU:HD11	1:A:81:LEU:CA	0.40	2.46	20	1
1:A:133:ARG:HD3	1:A:134:LEU:N	0.40	2.31	3	1
1:A:133:ARG:HD2	1:A:134:LEU:N	0.40	2.31	13	1
1:A:74:LEU:HB3	1:A:106:GLN:CG	0.40	2.47	17	1
1:A:159:TYR:O	1:A:163:GLU:HG2	0.40	2.16	20	1
1:A:64:GLU:HB2	1:A:68:LYS:CE	0.40	2.47	3	1
1:A:30:CYS:HB3	1:A:98:ASP:CG	0.40	2.42	14	1
1:A:52:VAL:HA	1:A:59:GLY:CA	0.40	2.46	15	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	192/199 (96%)	168±2 (87±1%)	21±2 (11±1%)	4±1 (2±1%)	8	49
All	All	3840/3980 (96%)	3350 (87%)	413 (11%)	77 (2%)	8	49

All 10 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	101	PRO	20
1	A	127	PRO	20
1	A	198	LEU	8
1	A	143	ARG	7
1	A	144	VAL	6
1	A	142	GLY	5
1	A	86	VAL	5
1	A	89	VAL	4
1	A	182	GLY	1
1	A	181	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/170 (98%)	121±3 (72±2%)	46±3 (28±2%)	1	20
All	All	3340/3400 (98%)	2411 (72%)	929 (28%)	1	20

All 90 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	14	LYS	20
1	A	15	ILE	20
1	A	17	PHE	20
1	A	18	VAL	20
1	A	37	TYR	20
1	A	42	LEU	20
1	A	62	LEU	20
1	A	78	LEU	20
1	A	81	LEU	20
1	A	88	LYS	20
1	A	89	VAL	20
1	A	113	ARG	20
1	A	119	LEU	20
1	A	120	LEU	20
1	A	131	THR	20
1	A	134	LEU	20
1	A	147	ASN	20
1	A	165	VAL	20
1	A	178	VAL	20
1	A	198	LEU	20
1	A	12	LYS	19
1	A	187	VAL	19
1	A	106	GLN	18
1	A	190	GLN	18
1	A	74	LEU	17
1	A	175	VAL	17
1	A	135	LEU	16
1	A	162	THR	16
1	A	26	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	153	LYS	15
1	A	155	LEU	15
1	A	181	GLU	15
1	A	102	ARG	15
1	A	47	LEU	14
1	A	144	VAL	14
1	A	10	LEU	14
1	A	58	ARG	14
1	A	130	MET	14
1	A	105	GLN	13
1	A	148	GLU	13
1	A	71	LEU	13
1	A	160	LYS	13
1	A	68	LYS	11
1	A	48	LEU	11
1	A	133	ARG	11
1	A	34	VAL	10
1	A	61	LYS	9
1	A	93	LYS	8
1	A	151	ILE	8
1	A	152	LYS	8
1	A	109	GLU	7
1	A	114	ILE	6
1	A	76	THR	6
1	A	85	MET	6
1	A	143	ARG	6
1	A	121	LEU	5
1	A	33	ILE	5
1	A	70	GLN	5
1	A	9	LYS	4
1	A	83	ASP	4
1	A	199	LYS	4
1	A	29	GLN	4
1	A	53	SER	4
1	A	92	SER	4
1	A	49	ARG	4
1	A	103	GLU	3
1	A	52	VAL	3
1	A	72	VAL	3
1	A	137	ARG	3
1	A	97	ILE	3
1	A	195	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	32	LYS	2
1	A	172	ARG	2
1	A	128	GLU	2
1	A	13	THR	2
1	A	184	VAL	2
1	A	129	THR	2
1	A	185	ASP	1
1	A	179	ASN	1
1	A	77	VAL	1
1	A	90	ASN	1
1	A	194	HIS	1
1	A	136	LYS	1
1	A	82	ARG	1
1	A	156	GLU	1
1	A	154	ARG	1
1	A	6	MET	1
1	A	145	ASP	1
1	A	35	GLN	1
1	A	149	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `cs_list`

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	2300
Number of shifts mapped to atoms	2300
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	16

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	188	-1.58 ± 0.11	Should be checked
$^{13}\text{C}_\beta$	163	-0.99 ± 0.13	Should be checked
$^{13}\text{C}'$	189	-1.47 ± 0.16	Should be applied
^{15}N	186	-0.66 ± 0.24	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 85%, i.e. 2258 atoms were assigned a chemical shift out of a possible 2664. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	958/977 (98%)	395/401 (99%)	377/388 (97%)	186/188 (99%)
Sidechain	1254/1558 (80%)	868/1007 (86%)	386/485 (80%)	0/66 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	46/129 (36%)	46/61 (75%)	0/64 (0%)	0/4 (0%)
Overall	2258/2664 (85%)	1309/1469 (89%)	763/937 (81%)	186/258 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2258 atoms were assigned a chemical shift out of a possible 2664. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	958/977 (98%)	395/401 (99%)	377/388 (97%)	186/188 (99%)
Sidechain	1254/1558 (80%)	868/1007 (86%)	386/485 (80%)	0/66 (0%)
Aromatic	46/129 (36%)	46/61 (75%)	0/64 (0%)	0/4 (0%)
Overall	2258/2664 (85%)	1309/1469 (89%)	763/937 (81%)	186/258 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

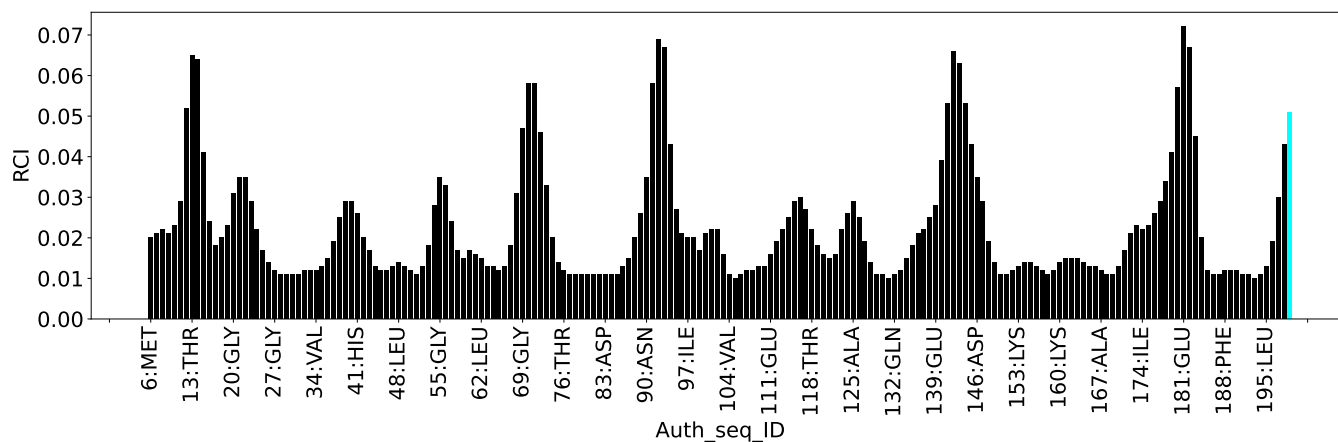
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	13	THR	HG1	5.33	0.08 – 2.19	19.9
1	A	44	THR	HG1	4.76	0.08 – 2.19	17.2
1	A	140	THR	HG1	4.76	0.08 – 2.19	17.2
1	A	28	THR	HG1	4.36	0.08 – 2.19	15.3
1	A	157	THR	HG1	4.34	0.08 – 2.19	15.2
1	A	162	THR	HG1	4.04	0.08 – 2.19	13.8
1	A	32	LYS	HE3	4.62	1.92 – 3.89	8.7
1	A	49	ARG	HD3	1.11	1.81 – 4.39	-7.7
1	A	122	TYR	HE1	8.42	5.59 – 7.82	7.7
1	A	54	SER	HB2	2.13	2.61 – 5.13	-6.9
1	A	137	ARG	HH21	9.31	4.81 – 8.80	6.3
1	A	177	LYS	HE3	4.13	1.92 – 3.89	6.2
1	A	176	ARG	HH11	9.40	4.72 – 9.08	5.7
1	A	102	ARG	HD3	4.53	1.81 – 4.39	5.5
1	A	60	LYS	HE3	3.95	1.92 – 3.89	5.3
1	A	190	GLN	HB2	3.32	0.80 – 3.29	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3005
Intra-residue ($ i-j =0$)	972
Sequential ($ i-j =1$)	778
Medium range ($ i-j >1$ and $ i-j <5$)	598
Long range ($ i-j \geq 5$)	657
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	350
Number of unmapped restraints	0
Number of restraints per residue	16.9
Number of long range restraints per residue ¹	3.3

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)	119.5	0.2
0.2-0.5 (Medium)	122.2	0.5
>0.5 (Large)	210.4	5.21

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)	50.1	6.62
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

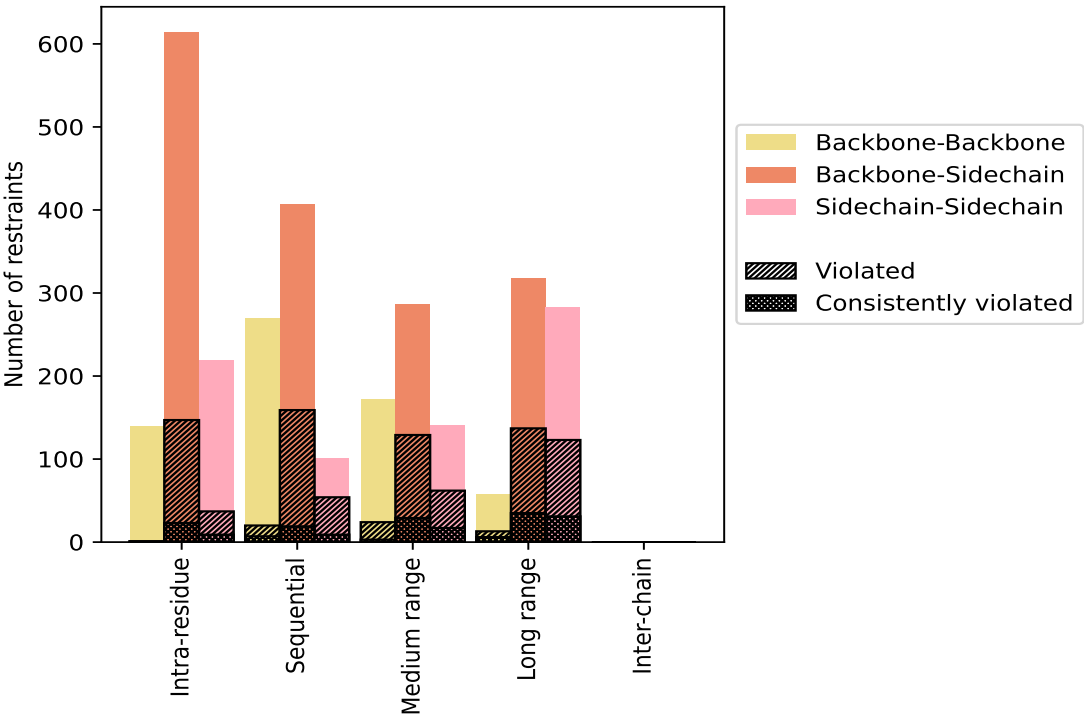
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	972	32.3	185	19.0	6.2	33	3.4	1.1
Backbone-Backbone	139	4.6	1	0.7	0.0	1	0.7	0.0
Backbone-Sidechain	614	20.4	147	23.9	4.9	23	3.7	0.8
Sidechain-Sidechain	219	7.3	37	16.9	1.2	9	4.1	0.3
Sequential ($i-j =1$)	778	25.9	233	29.9	7.8	35	4.5	1.2
Backbone-Backbone	270	9.0	20	7.4	0.7	7	2.6	0.2
Backbone-Sidechain	407	13.5	159	39.1	5.3	19	4.7	0.6
Sidechain-Sidechain	101	3.4	54	53.5	1.8	9	8.9	0.3
Medium range ($i-j >1$ & $i-j <5$)	598	19.9	215	36.0	7.2	49	8.2	1.6
Backbone-Backbone	172	5.7	24	14.0	0.8	3	1.7	0.1
Backbone-Sidechain	286	9.5	129	45.1	4.3	29	10.1	1.0
Sidechain-Sidechain	140	4.7	62	44.3	2.1	17	12.1	0.6
Long range ($i-j \geq 5$)	657	21.9	273	41.6	9.1	72	11.0	2.4
Backbone-Backbone	57	1.9	13	22.8	0.4	6	10.5	0.2
Backbone-Sidechain	317	10.5	137	43.2	4.6	35	11.0	1.2
Sidechain-Sidechain	283	9.4	123	43.5	4.1	31	11.0	1.0
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	3005	100.0	906	30.1	30.1	189	6.3	6.3
Backbone-Backbone	638	21.2	58	9.1	1.9	17	2.7	0.6
Backbone-Sidechain	1624	54.0	572	35.2	19.0	106	6.5	3.5
Sidechain-Sidechain	743	24.7	276	37.1	9.2	66	8.9	2.2

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	94	101	120	145	0	460	0.6	2.95	0.51	0.44
2	85	114	109	138	0	446	0.63	3.82	0.54	0.47
3	89	112	117	149	0	467	0.6	3.55	0.53	0.42
4	94	110	120	146	0	470	0.61	3.82	0.51	0.48
5	88	113	116	152	0	469	0.64	5.21	0.55	0.51
6	91	113	114	151	0	469	0.62	3.96	0.54	0.45
7	89	96	114	151	0	450	0.56	2.37	0.46	0.43
8	88	102	113	144	0	447	0.55	2.27	0.45	0.4
9	94	99	115	145	0	453	0.6	3.38	0.52	0.45
10	87	108	110	159	0	464	0.61	4.13	0.54	0.44

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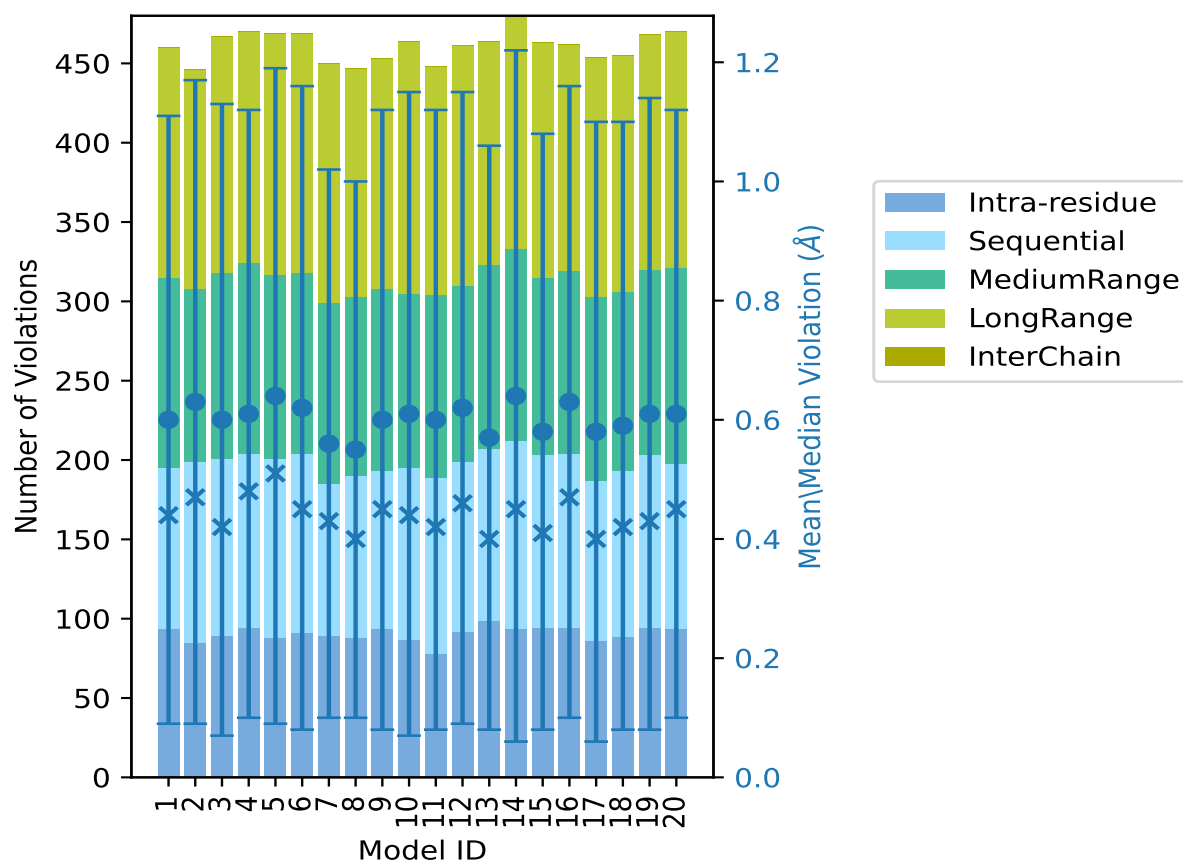
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	78	111	115	144	0	448	0.6	3.01	0.52	0.42
12	92	107	111	151	0	461	0.62	3.98	0.53	0.46
13	99	108	116	141	0	464	0.57	3.25	0.49	0.4
14	94	118	121	147	0	480	0.64	3.97	0.58	0.45
15	94	109	112	148	0	463	0.58	3.3	0.5	0.41
16	94	110	115	143	0	462	0.63	3.31	0.53	0.47
17	86	101	116	151	0	454	0.58	3.03	0.52	0.4
18	89	104	113	149	0	455	0.59	2.97	0.51	0.42
19	94	109	117	148	0	468	0.61	3.81	0.53	0.43
20	94	104	123	149	0	470	0.61	2.88	0.51	0.45

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

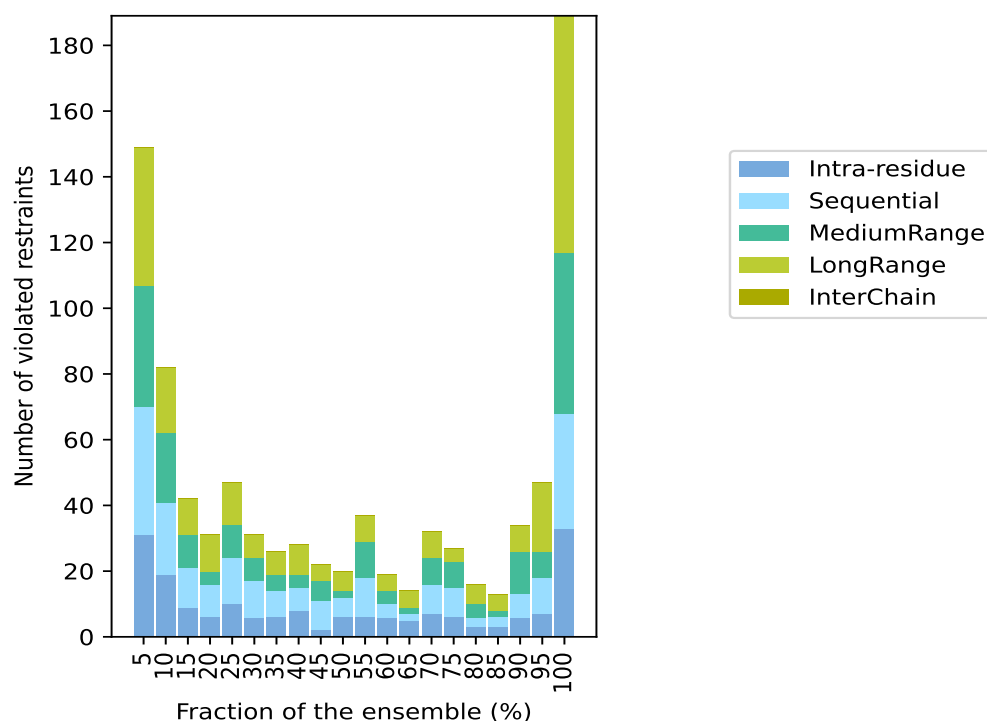
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2099(IR:787, SQ:545, MR:383, LR:384, IC:0) restraints are 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	%
31	39	37	42	0	149	1	5.0
19	22	21	20	0	82	2	10.0
9	12	10	11	0	42	3	15.0
6	10	4	11	0	31	4	20.0
10	14	10	13	0	47	5	25.0
6	11	7	7	0	31	6	30.0
6	8	5	7	0	26	7	35.0
8	7	4	9	0	28	8	40.0
2	9	6	5	0	22	9	45.0
6	6	2	6	0	20	10	50.0
6	12	11	8	0	37	11	55.0
6	4	4	5	0	19	12	60.0
5	2	2	5	0	14	13	65.0
7	9	8	8	0	32	14	70.0
6	9	8	4	0	27	15	75.0
3	3	4	6	0	16	16	80.0
3	3	2	5	0	13	17	85.0
6	7	13	8	0	34	18	90.0
7	11	8	21	0	47	19	95.0
33	35	49	72	0	189	20	100.0

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

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

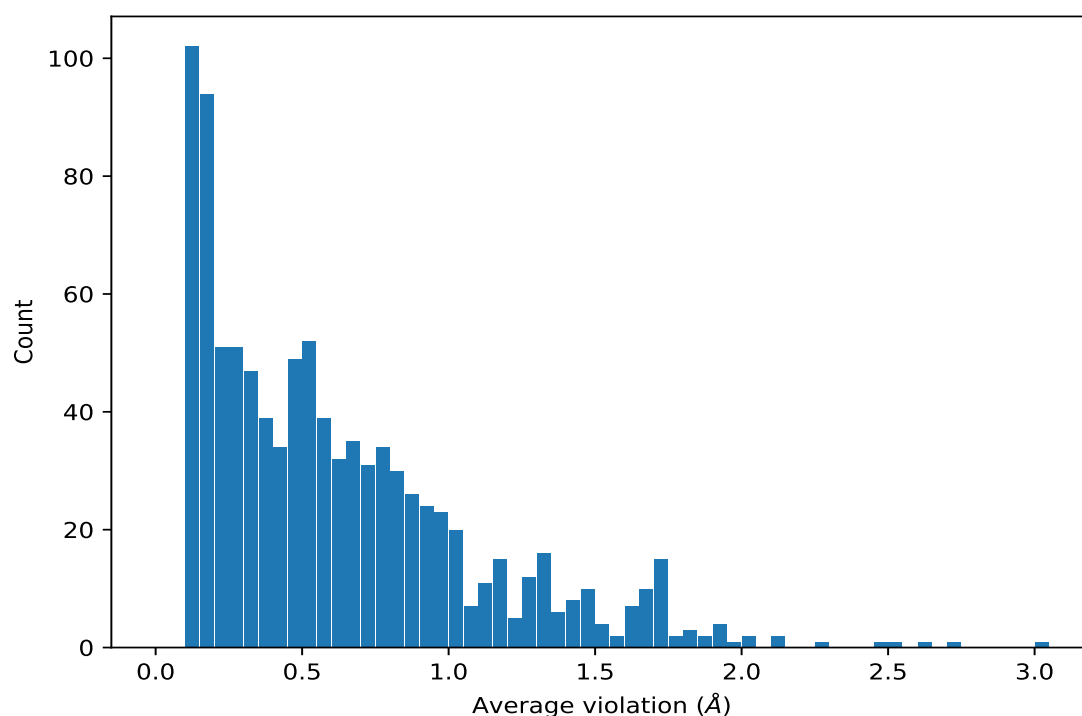
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	20	1.93	0.57	2.03
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	20	1.92	0.67	1.68
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	20	1.86	0.29	1.9
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	20	1.83	0.1	1.84
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	20	1.83	0.1	1.84
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	20	1.77	0.8	1.58
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD11	20	1.74	0.94	1.9
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	20	1.74	0.94	1.9
(4,219)	1:65:A:ILE:HA	1:72:A:VAL:HG22	20	1.74	0.94	1.9
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD23	20	1.74	0.94	1.9
(4,219)	1:65:A:ILE:HA	1:72:A:VAL:HG21	20	1.74	0.94	1.9
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD22	20	1.74	0.94	1.9
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	20	1.7	0.26	1.58
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	20	1.7	0.24	1.77
(4,147)	1:84:A:ALA:HB3	1:15:A:ILE:HD12	20	1.7	0.24	1.77
(4,147)	1:84:A:ALA:HB1	1:15:A:ILE:HD12	20	1.7	0.24	1.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,147)	1:197:A:ALA:HB1	1:121:A:LEU:HD21	20	1.7	0.24	1.77
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	20	1.67	0.04	1.67
(4,288)	1:93:A:LYS:H	1:16:A:ILE:HG13	20	1.61	0.07	1.6
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	20	1.61	0.07	1.6
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	20	1.5	0.57	1.32
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	20	1.49	0.03	1.5
(4,140)	1:34:A:VAL:HG22	1:33:A:ILE:HG22	20	1.49	0.23	1.55
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	20	1.49	0.23	1.55
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	20	1.49	0.23	1.55
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG22	20	1.49	0.23	1.55
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG23	20	1.49	0.23	1.55
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	20	1.49	0.15	1.5
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	20	1.47	0.07	1.48
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	20	1.34	0.26	1.4
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	20	1.32	0.27	1.25
(4,123)	1:144:A:VAL:HG12	1:22:A:PRO:HD2	20	1.32	0.27	1.25
(4,123)	1:144:A:VAL:HG11	1:22:A:PRO:HD2	20	1.32	0.27	1.25
(4,123)	1:144:A:VAL:HG13	1:22:A:PRO:HD2	20	1.32	0.27	1.25
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	20	1.32	0.18	1.37
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	20	1.31	0.08	1.3
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	20	1.29	0.71	1.37
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	20	1.29	0.29	1.38
(4,198)	1:77:A:VAL:HA	1:47:A:LEU:HB2	20	1.29	0.29	1.38
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	20	1.29	0.29	1.38
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HB2	20	1.29	0.29	1.38
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	20	1.27	0.24	1.32
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	20	1.25	0.03	1.27
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	20	1.22	0.35	1.1
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	20	1.21	0.15	1.25
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	20	1.21	0.07	1.21
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	20	1.21	0.23	1.18
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	20	1.19	0.03	1.18
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	20	1.19	0.06	1.19
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	20	1.18	0.18	1.21
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	20	1.16	0.41	1.35
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	20	1.14	0.12	1.13
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	20	1.13	0.08	1.15
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	20	1.12	0.06	1.12
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG22	20	1.12	0.1	1.12
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	20	1.12	0.1	1.12
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	20	1.12	0.1	1.12
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	20	1.07	0.17	1.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD1	20	1.07	0.17	1.12
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	20	1.05	0.68	0.94
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	20	1.04	0.14	0.98
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	20	1.02	0.04	1.01
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	20	1.0	0.29	1.05
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	20	1.0	0.19	1.08
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	20	0.99	0.21	0.97
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	20	0.98	0.05	0.98
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	20	0.98	0.05	0.98
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	20	0.95	0.45	1.08
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	20	0.93	0.13	0.99
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	20	0.93	0.31	0.9
(4,126)	1:144:A:VAL:HG11	1:154:A:ARG:HB3	20	0.93	0.31	0.9
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	20	0.93	0.31	0.9
(4,126)	1:144:A:VAL:HG12	1:22:A:PRO:HG2	20	0.93	0.31	0.9
(4,126)	1:144:A:VAL:HG11	1:70:A:GLN:HB2	20	0.93	0.31	0.9
(4,126)	1:144:A:VAL:HG13	1:70:A:GLN:HB2	20	0.93	0.31	0.9
(4,126)	1:144:A:VAL:HG12	1:154:A:ARG:HB3	20	0.93	0.31	0.9
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	20	0.93	0.33	1.04
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	20	0.91	0.09	0.94
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	20	0.9	0.37	1.08
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	20	0.9	0.47	1.16
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	20	0.89	0.15	0.92
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	20	0.88	0.19	0.86
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	20	0.87	0.04	0.88
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	20	0.86	0.68	0.7
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	20	0.85	0.38	0.77
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	20	0.84	0.29	0.84
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	20	0.83	0.19	0.82
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	20	0.83	0.19	0.82
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD11	20	0.83	0.19	0.82
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD12	20	0.83	0.19	0.82
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD13	20	0.83	0.19	0.82
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	20	0.83	0.23	0.82
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	20	0.82	0.13	0.81
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	20	0.81	0.18	0.83
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	20	0.81	0.21	0.75
(4,367)	1:13:A:THR:H	1:11:A:LYS:HG2	20	0.81	0.21	0.75
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	20	0.8	0.13	0.82
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	20	0.8	0.13	0.82
(4,133)	1:175:A:VAL:HG23	1:169:A:TYR:HD1	20	0.8	0.13	0.82
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	20	0.8	0.17	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	20	0.8	0.35	0.74
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	20	0.79	0.01	0.79
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	20	0.77	0.02	0.78
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	20	0.77	0.12	0.79
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	20	0.76	0.43	1.05
(4,10)	1:71:A:LEU:HG	1:65:A:ILE:HG23	20	0.76	0.29	0.72
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	20	0.76	0.29	0.72
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	20	0.76	0.29	0.72
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	20	0.75	0.14	0.78
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	20	0.74	0.03	0.74
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	20	0.73	0.05	0.73
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	20	0.73	0.05	0.73
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	20	0.73	0.14	0.76
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	20	0.72	0.2	0.76
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	20	0.72	0.22	0.78
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	20	0.71	0.02	0.71
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	20	0.71	0.09	0.74
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	20	0.7	0.19	0.76
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	20	0.7	0.02	0.7
(4,273)	1:167:A:ALA:HB1	1:164:A:PRO:HD2	20	0.7	0.02	0.7
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	20	0.7	0.26	0.66
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	20	0.68	0.08	0.67
(4,32)	1:113:A:ARG:HG3	1:113:A:ARG:HA	20	0.68	0.08	0.67
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	20	0.68	0.0	0.68
(4,399)	1:98:A:ASP:H	1:96:A:LEU:HA	20	0.67	0.04	0.66
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	20	0.67	0.04	0.66
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	20	0.67	0.08	0.65
(4,387)	1:99:A:GLY:H	1:43:A:SER:HA	20	0.67	0.08	0.65
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	20	0.66	0.03	0.67
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	20	0.66	0.03	0.67
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	20	0.64	0.75	0.16
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	20	0.63	0.19	0.56
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	20	0.61	0.05	0.6
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	20	0.61	0.03	0.61
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	20	0.6	0.1	0.62
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	20	0.59	0.14	0.68
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	20	0.58	0.34	0.65
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	20	0.58	0.21	0.62
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	20	0.57	0.06	0.57
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	20	0.57	0.55	0.17
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	20	0.56	0.0	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	20	0.56	0.0	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG21	20	0.56	0.0	0.56
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	20	0.56	0.21	0.63
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	20	0.56	0.21	0.63
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	20	0.56	0.14	0.52
(4,74)	1:10:A:LEU:HD21	1:95:A:PHE:HE2	20	0.56	0.14	0.52
(4,74)	1:10:A:LEU:HD22	1:95:A:PHE:HE2	20	0.56	0.14	0.52
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	20	0.55	0.09	0.53
(4,377)	1:172:A:ARG:H	1:117:A:PRO:HB3	20	0.55	0.09	0.53
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	20	0.53	0.04	0.53
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	20	0.52	0.14	0.58
(4,347)	1:90:A:ASN:H	1:9:A:LYS:HG2	20	0.52	0.14	0.58
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	20	0.52	0.41	0.31
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	20	0.52	0.41	0.31
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	20	0.51	0.13	0.52
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	20	0.51	0.13	0.52
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	20	0.51	0.07	0.54
(4,313)	1:190:A:GLN:H	1:186:A:SER:HA	20	0.51	0.07	0.54
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	20	0.51	0.05	0.5
(4,152)	1:167:A:ALA:HB3	1:170:A:GLU:HB2	20	0.51	0.05	0.5
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	20	0.5	0.06	0.51
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG23	20	0.5	0.06	0.51
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	20	0.5	0.22	0.47
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG22	20	0.5	0.22	0.47
(4,280)	1:179:A:ASN:H	1:178:A:VAL:HG11	20	0.5	0.22	0.47
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	20	0.49	0.21	0.44
(4,335)	1:83:A:ASP:H	1:86:A:VAL:HG21	20	0.49	0.21	0.44
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	20	0.48	0.08	0.5
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	20	0.46	0.14	0.44
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	20	0.46	0.08	0.49
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	20	0.46	0.11	0.43
(4,250)	1:34:A:VAL:HB	1:31:A:GLU:HA	20	0.46	0.11	0.43
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	20	0.46	0.02	0.46
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	20	0.45	0.22	0.4
(4,298)	1:81:A:LEU:HG	1:81:A:LEU:H	20	0.45	0.22	0.4
(4,298)	1:81:A:LEU:H	1:84:A:ALA:HB1	20	0.45	0.22	0.4
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	20	0.44	0.1	0.42
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	20	0.44	0.17	0.4
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	20	0.43	0.04	0.44
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	20	0.43	0.1	0.45
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	20	0.42	0.01	0.42
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	20	0.41	0.08	0.41
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	20	0.41	0.04	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	20	0.4	0.13	0.42
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	20	0.4	0.13	0.42
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	20	0.39	0.09	0.4
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	20	0.39	0.04	0.38
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	20	0.37	0.58	0.14
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	20	0.37	0.72	0.2
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG23	20	0.37	0.72	0.2
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG21	20	0.37	0.72	0.2
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	20	0.37	0.16	0.42
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	20	0.37	0.05	0.38
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	20	0.36	0.02	0.36
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	20	0.36	0.02	0.36
(4,57)	1:19:A:VAL:HG12	1:19:A:VAL:HB	20	0.36	0.02	0.36
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	20	0.36	0.04	0.36
(4,266)	1:108:A:GLU:HA	1:108:A:GLU:HB2	20	0.36	0.04	0.36
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	20	0.36	0.2	0.32
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	20	0.34	0.09	0.38
(4,16)	1:195:A:LEU:HD23	1:198:A:LEU:HB3	20	0.34	0.09	0.38
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG22	20	0.34	0.07	0.36
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	20	0.34	0.07	0.36
(4,344)	1:39:A:TYR:H	1:34:A:VAL:HG11	20	0.34	0.09	0.34
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	20	0.34	0.09	0.34
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	20	0.33	0.03	0.33
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	20	0.33	0.07	0.34
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	20	0.33	0.36	0.22
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	20	0.31	0.7	0.16
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	20	0.31	0.03	0.32
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	20	0.31	0.04	0.32
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	20	0.31	0.04	0.32
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	20	0.3	0.03	0.29
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	20	0.29	0.05	0.3
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	20	0.28	0.29	0.21
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	20	0.28	0.03	0.28
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	20	0.27	0.09	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	20	0.27	0.09	0.22
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	20	0.27	0.29	0.2
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	20	0.27	0.0	0.27
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	20	0.27	0.15	0.21
(4,269)	1:132:A:GLN:HA	1:132:A:GLN:HB2	20	0.27	0.15	0.21
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	20	0.26	0.08	0.3
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	20	0.26	0.26	0.2
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	20	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	20	0.26	0.01	0.25
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	20	0.25	0.02	0.26
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	20	0.25	0.01	0.25
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	20	0.25	0.05	0.24
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	20	0.24	0.05	0.24
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	20	0.24	0.06	0.22
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	20	0.23	0.01	0.24
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	20	0.23	0.03	0.24
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	20	0.23	0.03	0.23
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	20	0.21	0.03	0.2
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	20	0.21	0.08	0.18
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	20	0.21	0.02	0.21
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	20	0.21	0.03	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	20	0.2	0.03	0.2
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	20	0.2	0.02	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	20	0.2	0.01	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	20	0.19	0.01	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	20	0.19	0.03	0.19
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	20	0.19	0.03	0.2
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	20	0.19	0.04	0.18
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	20	0.18	0.05	0.18
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	20	0.18	0.03	0.18
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	20	0.18	0.03	0.18
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	20	0.17	0.02	0.18
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	20	0.17	0.04	0.16
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	20	0.17	0.07	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	20	0.17	0.02	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	20	0.17	0.02	0.17
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	20	0.16	0.02	0.16
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	20	0.15	0.01	0.15
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	20	0.15	0.02	0.16
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	20	0.15	0.01	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	20	0.15	0.02	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	20	0.14	0.01	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	20	0.14	0.01	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	20	0.14	0.01	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	20	0.13	0.02	0.14
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	20	0.12	0.01	0.12
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	19	1.73	0.54	1.96
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	19	1.65	0.08	1.66
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	19	1.64	0.12	1.69
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	19	1.64	0.83	1.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	19	1.34	0.18	1.35
(4,76)	1:104:A:VAL:HG12	1:166:A:ILE:HA	19	1.34	0.18	1.35
(4,76)	1:104:A:VAL:HG11	1:160:A:LYS:HE3	19	1.34	0.18	1.35
(4,76)	1:10:A:LEU:HD22	1:86:A:VAL:HA	19	1.34	0.18	1.35
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	19	1.29	0.03	1.3
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	19	1.05	0.75	1.67
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	19	1.04	0.55	1.14
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	19	0.98	0.17	0.97
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	19	0.85	0.18	0.92
(4,131)	1:77:A:VAL:HG23	1:100:A:TYR:HE1	19	0.85	0.18	0.92
(4,131)	1:77:A:VAL:HG22	1:100:A:TYR:HE1	19	0.85	0.18	0.92
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	19	0.8	0.12	0.83
(4,80)	1:78:A:LEU:HD22	1:81:A:LEU:HD23	19	0.77	0.17	0.83
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	19	0.77	0.17	0.83
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	19	0.77	0.17	0.83
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	19	0.72	0.18	0.7
(4,108)	1:178:A:VAL:HG12	1:190:A:GLN:HG3	19	0.72	0.18	0.7
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	19	0.72	0.31	0.82
(4,211)	1:67:A:GLU:HG2	1:68:A:LYS:HE2	19	0.72	0.31	0.82
(4,81)	1:10:A:LEU:HD22	1:85:A:MET:HA	19	0.68	0.2	0.74
(4,81)	1:10:A:LEU:HD21	1:85:A:MET:HA	19	0.68	0.2	0.74
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	19	0.68	0.2	0.74
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	19	0.68	0.07	0.67
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	19	0.68	0.07	0.67
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	19	0.66	0.97	0.25
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	19	0.64	1.08	0.29
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	19	0.57	0.19	0.56
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	19	0.55	0.26	0.46
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	19	0.52	0.31	0.41
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	19	0.52	0.14	0.51
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG23	19	0.52	0.14	0.51
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	19	0.5	0.27	0.5
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	19	0.5	0.27	0.5
(4,35)	1:61:A:LYS:HD2	1:58:A:ARG:HA	19	0.5	0.27	0.5
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	19	0.48	0.14	0.51
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD1	19	0.48	0.14	0.51
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	19	0.48	0.14	0.51
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	19	0.46	0.4	0.21
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	19	0.45	0.13	0.42
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	19	0.45	0.13	0.42
(4,369)	1:183:A:SER:H	1:187:A:VAL:HG11	19	0.45	0.13	0.42
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG23	19	0.45	0.13	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	19	0.43	0.05	0.46
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	19	0.41	0.15	0.37
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG21	19	0.41	0.15	0.37
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	19	0.4	0.11	0.41
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	19	0.4	0.11	0.41
(4,44)	1:160:A:LYS:HA	1:164:A:PRO:HD2	19	0.4	0.11	0.41
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	19	0.4	0.3	0.27
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	19	0.39	0.11	0.38
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	19	0.39	0.15	0.35
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	19	0.33	0.15	0.29
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	19	0.32	0.16	0.29
(4,339)	1:80:A:MET:H	1:84:A:ALA:HB1	19	0.32	0.16	0.29
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	19	0.31	0.33	0.2
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	19	0.29	0.11	0.34
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	19	0.27	0.13	0.24
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	19	0.27	0.13	0.24
(4,222)	1:67:A:GLU:HG2	1:64:A:GLU:HA	19	0.27	0.13	0.24
(4,222)	1:48:A:LEU:HA	1:51:A:GLU:HG2	19	0.27	0.13	0.24
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HB3	19	0.24	0.08	0.24
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	19	0.24	0.08	0.24
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	19	0.24	0.04	0.24
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	19	0.23	0.07	0.21
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	19	0.22	0.03	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	19	0.19	0.04	0.21
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	19	0.18	0.02	0.17
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	19	0.16	0.03	0.16
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	19	0.14	0.05	0.12
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	19	0.14	0.01	0.14
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	19	0.13	0.02	0.13
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	18	1.51	0.63	1.78
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	18	1.26	0.07	1.25
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	18	0.93	0.28	0.94
(4,107)	1:129:A:THR:HG23	1:181:A:GLU:HG2	18	0.93	0.28	0.94
(4,107)	1:44:A:THR:HG22	1:77:A:VAL:HB	18	0.93	0.28	0.94
(4,107)	1:129:A:THR:HG21	1:128:A:GLU:HG3	18	0.93	0.28	0.94
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	18	0.83	0.25	0.75
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	18	0.81	0.22	0.82
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	18	0.81	0.22	0.82
(4,50)	1:88:A:LYS:HG3	1:88:A:LYS:HE2	18	0.71	0.25	0.86
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	18	0.71	0.25	0.86
(4,50)	1:160:A:LYS:HG3	1:160:A:LYS:HE2	18	0.71	0.25	0.86
(4,66)	1:86:A:VAL:HG12	1:6:A:MET:H	18	0.69	0.27	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	18	0.69	0.27	0.72
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	18	0.69	0.27	0.72
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD22	18	0.69	0.27	0.72
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	18	0.64	0.54	0.57
(4,20)	1:74:A:LEU:HG	1:105:A:GLN:HB2	18	0.64	0.54	0.57
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	18	0.63	0.08	0.6
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	18	0.63	0.08	0.6
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG13	18	0.63	0.08	0.6
(4,88)	1:76:A:THR:HG23	1:62:A:LEU:HB2	18	0.61	0.33	0.55
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	18	0.61	0.33	0.55
(4,88)	1:76:A:THR:HG22	1:62:A:LEU:HB2	18	0.61	0.33	0.55
(4,88)	1:76:A:THR:HG23	1:73:A:PRO:HB3	18	0.61	0.33	0.55
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	18	0.56	0.15	0.59
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	18	0.56	0.19	0.66
(4,82)	1:10:A:LEU:HD21	1:116:A:GLN:HG2	18	0.56	0.19	0.66
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	18	0.54	0.25	0.5
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	18	0.54	0.25	0.5
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	18	0.51	0.4	0.44
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	18	0.41	0.19	0.43
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	18	0.41	0.07	0.41
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD22	18	0.41	0.07	0.41
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	18	0.4	0.1	0.38
(4,237)	1:171:A:LYS:HB2	1:168:A:PHE:HA	18	0.4	0.1	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	18	0.38	0.02	0.38
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	18	0.33	0.09	0.32
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	18	0.32	0.15	0.34
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	18	0.28	0.11	0.26
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	18	0.26	0.05	0.27
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	18	0.26	0.14	0.2
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	18	0.24	0.01	0.24
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	18	0.24	0.21	0.16
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	18	0.2	0.3	0.13
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	18	0.2	0.05	0.18
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	18	0.19	0.04	0.2
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	18	0.18	0.06	0.16
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	18	0.18	0.05	0.18
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	18	0.17	0.02	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	18	0.17	0.01	0.17
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	18	0.16	0.05	0.14
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	18	0.15	0.02	0.16
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	17	1.08	0.03	1.09
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	17	0.79	0.32	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	17	0.66	0.36	0.67
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	17	0.65	0.31	0.57
(4,199)	1:8:A:GLU:HG2	1:6:A:MET:H	17	0.65	0.31	0.57
(4,199)	1:156:A:GLU:HG3	1:152:A:LYS:HD2	17	0.65	0.31	0.57
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	17	0.65	0.16	0.69
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	17	0.58	0.33	0.75
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	17	0.55	0.09	0.53
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	17	0.53	0.25	0.65
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	17	0.31	0.09	0.32
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	17	0.18	0.03	0.19
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	17	0.15	0.02	0.15
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	17	0.13	0.02	0.12
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	17	0.13	0.01	0.13
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	16	0.96	0.24	1.0
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	16	0.75	0.23	0.88
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	16	0.51	0.15	0.5
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	16	0.45	0.16	0.5
(4,24)	1:47:A:LEU:HG	1:44:A:THR:HA	16	0.45	0.16	0.5
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	16	0.4	0.12	0.42
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	16	0.24	0.14	0.18
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	16	0.23	0.06	0.22
(1,91)	1:134:A:LEU:HD13	1:135:A:LEU:HA	16	0.23	0.06	0.22
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	16	0.2	0.11	0.15
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	16	0.2	0.06	0.2
(4,328)	1:153:A:LYS:H	1:152:A:LYS:HA	16	0.2	0.06	0.2
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	16	0.19	0.05	0.18
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	16	0.18	0.02	0.18
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	16	0.17	0.03	0.16
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	16	0.16	0.03	0.17
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	16	0.16	0.03	0.16
(4,163)	1:166:A:ILE:HG21	1:170:A:GLU:HA	16	0.16	0.03	0.16
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	16	0.16	0.05	0.15
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	16	0.14	0.02	0.14
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	15	1.36	0.06	1.4
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	15	1.28	0.07	1.27
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	15	1.26	0.03	1.25
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	15	1.08	0.26	1.12
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	15	0.99	0.1	1.0
(4,234)	1:186:A:SER:HB2	1:185:A:ASP:HB2	15	0.99	0.1	1.0
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	15	0.97	0.8	1.55
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	15	0.94	1.14	0.53
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	15	0.87	0.24	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,143)	1:89:A:VAL:HG22	1:10:A:LEU:HB2	15	0.87	0.24	0.8
(4,143)	1:89:A:VAL:HG22	1:88:A:LYS:HD2	15	0.87	0.24	0.8
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	15	0.81	0.5	0.87
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	15	0.79	0.03	0.79
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG22	15	0.79	0.03	0.79
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG23	15	0.79	0.03	0.79
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	15	0.78	0.69	0.23
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	15	0.64	0.31	0.65
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	15	0.61	0.18	0.68
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	15	0.55	0.2	0.65
(4,322)	1:86:A:VAL:H	1:82:A:ARG:HG2	15	0.55	0.2	0.65
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB1	15	0.55	0.2	0.65
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	15	0.52	0.15	0.49
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	15	0.51	0.32	0.32
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	15	0.45	0.38	0.2
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	15	0.34	0.39	0.15
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	15	0.3	0.05	0.28
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	15	0.28	0.04	0.26
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	15	0.25	0.03	0.24
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	15	0.22	0.16	0.12
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	15	0.19	0.14	0.15
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	15	0.18	0.02	0.19
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	15	0.18	0.06	0.16
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	15	0.14	0.02	0.14
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	15	0.12	0.02	0.12
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	14	1.93	0.1	1.94
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	14	1.52	0.69	1.65
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	14	1.17	0.39	1.14
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	14	1.16	0.64	1.52
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	14	1.03	0.85	0.7
(1,97)	1:52:A:VAL:HG13	1:58:A:ARG:HD2	14	1.03	0.85	0.7
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG23	14	1.0	0.39	0.85
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	14	1.0	0.39	0.85
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	14	1.0	0.39	0.85
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG21	14	1.0	0.39	0.85
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	14	0.98	0.18	1.01
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	14	0.98	0.18	1.01
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	14	0.93	0.37	0.98
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	14	0.91	0.57	1.22
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	14	0.79	0.06	0.78
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	14	0.78	0.7	0.28
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	14	0.72	0.23	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	14	0.7	0.01	0.7
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	14	0.68	0.02	0.68
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	14	0.56	0.16	0.54
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	14	0.55	0.4	0.44
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	14	0.48	0.18	0.47
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	14	0.45	0.27	0.68
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	14	0.37	0.37	0.23
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD13	14	0.37	0.37	0.23
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD12	14	0.37	0.37	0.23
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	14	0.34	0.2	0.29
(4,286)	1:151:A:ILE:H	1:153:A:LYS:HE2	14	0.34	0.2	0.29
(4,286)	1:163:A:GLU:H	1:160:A:LYS:HE2	14	0.34	0.2	0.29
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE1	14	0.34	0.09	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	14	0.34	0.09	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	14	0.34	0.09	0.31
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	14	0.32	0.14	0.36
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	14	0.27	0.1	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	14	0.24	0.02	0.24
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	14	0.2	0.06	0.2
(4,97)	1:44:A:THR:HG22	1:100:A:TYR:HA	14	0.2	0.06	0.2
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	14	0.15	0.04	0.15
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	14	0.13	0.03	0.13
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	14	0.13	0.02	0.14
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	14	0.13	0.02	0.13
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	14	0.13	0.02	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	14	0.12	0.01	0.12
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	14	0.12	0.01	0.11
(4,169)	1:65:A:ILE:HD11	1:68:A:LYS:HD2	13	1.69	0.41	1.82
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	13	1.69	0.41	1.82
(4,169)	1:65:A:ILE:HD11	1:48:A:LEU:HB3	13	1.69	0.41	1.82
(4,169)	1:65:A:ILE:HD13	1:48:A:LEU:HB3	13	1.69	0.41	1.82
(4,169)	1:65:A:ILE:HD13	1:68:A:LYS:HD2	13	1.69	0.41	1.82
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	13	1.64	0.56	1.27
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	13	1.12	0.3	1.2
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	13	1.04	0.33	1.04
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	13	0.69	0.24	0.68
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	13	0.58	0.06	0.6
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	13	0.54	0.14	0.54
(4,401)	1:24:A:SER:H	1:130:A:MET:HE1	13	0.39	0.09	0.41
(4,401)	1:24:A:SER:H	1:130:A:MET:HE2	13	0.39	0.09	0.41
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	13	0.39	0.09	0.41
(4,401)	1:24:A:SER:H	1:134:A:LEU:HB2	13	0.39	0.09	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	13	0.38	0.1	0.39
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	13	0.31	0.08	0.31
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	13	0.31	0.08	0.31
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	13	0.17	0.04	0.18
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	13	0.15	0.03	0.15
(4,155)	1:105:A:GLN:HA	1:105:A:GLN:HG3	13	0.15	0.03	0.15
(4,155)	1:67:A:GLU:HA	1:67:A:GLU:HB3	13	0.15	0.03	0.15
(4,155)	1:8:A:GLU:HA	1:8:A:GLU:HG2	13	0.15	0.03	0.15
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	13	0.12	0.02	0.12
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	13	0.12	0.01	0.12
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	12	1.17	0.1	1.14
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	12	1.03	0.55	1.09
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	12	0.95	0.77	1.06
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	12	0.77	0.03	0.78
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	12	0.56	0.7	0.14
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	12	0.54	0.01	0.55
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	12	0.49	0.09	0.48
(4,301)	1:145:A:ASP:H	1:143:A:ARG:HD2	12	0.49	0.09	0.48
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	12	0.45	0.23	0.47
(4,370)	1:50:A:SER:H	1:80:A:MET:HE2	12	0.45	0.23	0.47
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	12	0.31	0.64	0.12
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	12	0.3	0.09	0.32
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	12	0.29	0.0	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	12	0.28	0.05	0.29
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	12	0.28	0.13	0.25
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	12	0.23	0.29	0.15
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	12	0.22	0.05	0.24
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	12	0.16	0.04	0.14
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	12	0.15	0.01	0.15
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	12	0.12	0.02	0.12
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	12	0.12	0.02	0.11
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	11	2.49	0.91	2.94
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	11	1.57	0.07	1.55
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	11	1.45	0.11	1.48
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	11	1.38	0.41	1.52
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	11	1.11	0.32	1.22
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	11	0.98	0.79	1.6
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	11	0.97	0.35	0.78
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	11	0.86	0.36	1.02
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	11	0.83	0.61	0.68
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	11	0.82	0.36	0.62
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	11	0.78	0.09	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG3	11	0.67	0.27	0.51
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	11	0.67	0.27	0.51
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	11	0.65	0.23	0.59
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	11	0.63	0.17	0.67
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	11	0.6	0.05	0.59
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	11	0.6	0.01	0.6
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	11	0.59	0.1	0.6
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	11	0.54	0.11	0.53
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	11	0.53	0.35	0.48
(4,170)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	11	0.53	0.35	0.48
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	11	0.52	0.36	0.36
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	11	0.51	0.24	0.64
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	11	0.5	0.16	0.58
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	11	0.48	0.19	0.45
(4,146)	1:161:A:ALA:HB1	1:162:A:THR:HG1	11	0.48	0.27	0.6
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	11	0.48	0.27	0.6
(4,146)	1:161:A:ALA:HB2	1:162:A:THR:HG1	11	0.48	0.27	0.6
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	11	0.41	0.21	0.46
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	11	0.31	0.02	0.31
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	11	0.3	0.1	0.3
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	11	0.27	0.1	0.26
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	11	0.25	0.05	0.26
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	11	0.16	0.06	0.14
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	11	0.15	0.02	0.14
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	11	0.15	0.03	0.14
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	11	0.13	0.02	0.12
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	11	0.12	0.02	0.13
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	11	0.12	0.02	0.12
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	11	0.12	0.01	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	11	0.11	0.01	0.11
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	10	1.68	0.36	1.56
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	10	1.13	0.08	1.13
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	10	0.98	0.21	1.1
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	10	0.95	0.54	0.76
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	10	0.76	0.35	0.86
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	10	0.69	0.4	0.56
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	10	0.57	0.02	0.57
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	10	0.52	0.14	0.59
(4,306)	1:143:A:ARG:H	1:138:A:GLY:HA3	10	0.52	0.14	0.59
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	10	0.51	0.09	0.53
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	10	0.37	0.11	0.42
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG12	10	0.37	0.11	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	10	0.28	0.04	0.29
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	10	0.25	0.09	0.21
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	10	0.19	0.03	0.21
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	10	0.19	0.16	0.14
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	10	0.18	0.05	0.18
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	10	0.13	0.02	0.13
(4,41)	1:35:A:GLN:HA	1:35:A:GLN:HG2	10	0.13	0.02	0.13
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	10	0.13	0.02	0.12
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	10	0.12	0.02	0.12
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	10	0.12	0.01	0.12
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	10	0.11	0.01	0.11
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	9	1.47	0.48	1.63
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	9	1.3	0.2	1.26
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	9	1.22	0.13	1.24
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	9	1.04	0.02	1.03
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	9	0.95	0.63	0.59
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	9	0.9	0.08	0.91
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	9	0.82	0.02	0.82
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	9	0.81	0.6	0.34
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	9	0.8	0.16	0.87
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	9	0.79	0.3	1.04
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	9	0.77	0.07	0.75
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	9	0.72	0.51	0.52
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	9	0.69	0.34	0.77
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	9	0.62	0.08	0.63
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	9	0.56	0.11	0.59
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	9	0.54	0.2	0.56
(4,83)	1:64:A:GLU:HA	1:68:A:LYS:HE3	9	0.54	0.2	0.56
(4,83)	1:8:A:GLU:HA	1:11:A:LYS:HE2	9	0.54	0.2	0.56
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	9	0.46	0.14	0.46
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	9	0.13	0.03	0.13
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	9	0.13	0.02	0.14
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	9	0.13	0.02	0.12
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	9	0.13	0.02	0.12
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	9	0.13	0.01	0.12
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	8	1.42	0.28	1.3
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	8	1.35	0.03	1.35
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	8	1.03	0.53	1.08
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	8	1.01	0.24	1.1
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	8	0.92	0.62	1.04
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	8	0.77	0.51	0.85
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	8	0.65	0.2	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	8	0.63	0.51	0.64
(1,81)	1:76:A:THR:HG23	1:58:A:ARG:HD2	8	0.63	0.43	0.64
(1,81)	1:76:A:THR:HG22	1:58:A:ARG:HD2	8	0.63	0.43	0.64
(1,81)	1:76:A:THR:HG21	1:58:A:ARG:HD2	8	0.63	0.43	0.64
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	8	0.57	0.33	0.76
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	8	0.48	0.26	0.35
(4,95)	1:76:A:THR:HG21	1:73:A:PRO:HG3	8	0.46	0.33	0.31
(4,95)	1:76:A:THR:HG23	1:58:A:ARG:HG2	8	0.46	0.33	0.31
(4,95)	1:76:A:THR:HG23	1:73:A:PRO:HG3	8	0.46	0.33	0.31
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	8	0.41	0.01	0.42
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	8	0.38	0.27	0.22
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	8	0.34	0.25	0.2
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	8	0.31	0.47	0.13
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG11	8	0.29	0.11	0.27
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	8	0.29	0.11	0.27
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	8	0.28	0.09	0.26
(4,101)	1:191:A:VAL:HG22	1:191:A:VAL:HA	8	0.25	0.04	0.24
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	8	0.25	0.04	0.24
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	8	0.24	0.09	0.26
(4,383)	1:23:A:GLY:H	1:26:A:LYS:HG3	8	0.24	0.09	0.26
(4,383)	1:23:A:GLY:H	1:134:A:LEU:HB3	8	0.24	0.09	0.26
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	8	0.16	0.06	0.15
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	8	0.16	0.04	0.15
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	8	0.15	0.01	0.15
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	8	0.13	0.02	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	8	0.12	0.01	0.12
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	8	0.12	0.02	0.12
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	8	0.12	0.01	0.12
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	8	0.11	0.01	0.11
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	7	2.12	0.2	2.16
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	7	1.71	0.01	1.71
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	7	1.44	1.19	1.84
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	7	1.16	0.66	1.57
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	7	1.06	0.82	1.02
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	7	0.93	0.09	0.95
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	7	0.78	0.43	0.63
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	7	0.72	0.45	0.73
(4,217)	1:47:A:LEU:HD13	1:43:A:SER:HB3	7	0.71	0.57	0.43
(4,217)	1:47:A:LEU:HD11	1:43:A:SER:HB3	7	0.71	0.57	0.43
(4,217)	1:47:A:LEU:HD12	1:43:A:SER:HB3	7	0.71	0.57	0.43
(4,217)	1:43:A:SER:HB3	1:42:A:LEU:HD12	7	0.71	0.57	0.43
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	7	0.6	0.6	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	7	0.54	0.08	0.54
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	7	0.48	0.11	0.55
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	7	0.44	0.15	0.45
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	7	0.43	0.11	0.39
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	7	0.31	0.09	0.25
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	7	0.28	0.11	0.26
(4,341)	1:80:A:MET:H	1:80:A:MET:HE3	7	0.28	0.11	0.26
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	7	0.26	0.03	0.27
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	7	0.24	0.11	0.19
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	7	0.22	0.07	0.26
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HG2	7	0.22	0.07	0.26
(4,243)	1:189:A:SER:HA	1:192:A:CYS:HB3	7	0.22	0.06	0.23
(4,243)	1:159:A:TYR:HA	1:163:A:GLU:HG3	7	0.22	0.06	0.23
(4,243)	1:159:A:TYR:HA	1:163:A:GLU:HG2	7	0.22	0.06	0.23
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	7	0.21	0.08	0.21
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG12	7	0.21	0.08	0.21
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	7	0.17	0.0	0.17
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	7	0.17	0.02	0.17
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	7	0.15	0.03	0.15
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	7	0.14	0.02	0.14
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	7	0.11	0.01	0.1
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	6	1.44	0.15	1.47
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	6	1.42	0.05	1.4
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	6	1.16	0.13	1.19
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	6	1.12	0.19	1.12
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	6	0.89	0.53	1.25
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	6	0.85	0.03	0.84
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	6	0.77	0.1	0.78
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	6	0.71	0.07	0.7
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	6	0.63	0.05	0.62
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	6	0.6	0.08	0.63
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	6	0.56	0.44	0.52
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	6	0.51	0.03	0.51
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	6	0.51	0.1	0.46
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	6	0.42	0.02	0.42
(4,92)	1:76:A:THR:HG21	1:80:A:MET:HG3	6	0.41	0.19	0.44
(4,92)	1:76:A:THR:HG21	1:79:A:ASP:HB2	6	0.41	0.19	0.44
(4,92)	1:76:A:THR:HG22	1:80:A:MET:HG3	6	0.41	0.19	0.44
(4,96)	1:76:A:THR:HG22	1:62:A:LEU:HD12	6	0.39	0.27	0.28
(4,96)	1:76:A:THR:HG23	1:62:A:LEU:HD12	6	0.39	0.27	0.28
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	6	0.33	0.11	0.29
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	6	0.32	0.04	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	6	0.3	0.15	0.24
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	6	0.27	0.1	0.27
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	6	0.19	0.06	0.21
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	6	0.19	0.01	0.18
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	6	0.16	0.02	0.16
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	6	0.14	0.02	0.15
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	6	0.14	0.02	0.14
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	6	0.13	0.02	0.13
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	6	0.12	0.02	0.12
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	6	0.12	0.01	0.13
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	6	0.12	0.02	0.12
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	6	0.11	0.01	0.11
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	6	0.1	0.0	0.1
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	5	2.26	1.33	1.27
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	5	1.7	0.01	1.7
(4,204)	1:28:A:THR:HA	1:29:A:GLN:HB3	5	1.42	0.03	1.43
(4,204)	1:157:A:THR:HA	1:160:A:LYS:HB3	5	1.42	0.03	1.43
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	5	1.39	0.06	1.38
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	5	1.29	0.03	1.29
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	5	1.02	0.21	1.01
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	5	0.98	0.72	1.56
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	5	0.95	0.41	1.08
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	5	0.91	0.0	0.91
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	5	0.89	0.37	1.03
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	5	0.88	0.03	0.9
(4,132)	1:175:A:VAL:HG23	1:166:A:ILE:H	5	0.86	0.35	1.01
(4,132)	1:19:A:VAL:HG22	1:166:A:ILE:H	5	0.86	0.35	1.01
(4,132)	1:184:A:VAL:HG22	1:188:A:PHE:HD2	5	0.86	0.35	1.01
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	5	0.85	0.32	0.97
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	5	0.83	0.01	0.83
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	5	0.82	0.03	0.8
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	5	0.77	0.08	0.78
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	5	0.65	0.06	0.65
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	5	0.54	0.07	0.54
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	5	0.5	0.02	0.49
(4,144)	1:89:A:VAL:HG23	1:6:A:MET:H	5	0.48	0.17	0.51
(4,144)	1:89:A:VAL:HG23	1:9:A:LYS:HG2	5	0.48	0.17	0.51
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	5	0.48	0.2	0.54
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	5	0.46	0.21	0.48
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	5	0.46	0.02	0.47
(4,296)	1:46:A:ASP:H	1:48:A:LEU:HD21	5	0.45	0.24	0.39
(4,296)	1:46:A:ASP:H	1:47:A:LEU:HD11	5	0.45	0.24	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,296)	1:46:A:ASP:H	1:47:A:LEU:HD13	5	0.45	0.24	0.39
(4,296)	1:46:A:ASP:H	1:48:A:LEU:HD11	5	0.45	0.24	0.39
(4,196)	1:131:A:THR:HA	1:134:A:LEU:HG	5	0.41	0.12	0.47
(4,196)	1:131:A:THR:HA	1:151:A:ILE:HG22	5	0.41	0.12	0.47
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	5	0.34	0.02	0.34
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	5	0.34	0.12	0.27
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	5	0.29	0.14	0.21
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	5	0.28	0.07	0.24
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	5	0.26	0.01	0.26
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	5	0.26	0.1	0.3
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	5	0.2	0.07	0.18
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	5	0.17	0.02	0.18
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	5	0.17	0.02	0.16
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	5	0.16	0.06	0.13
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	5	0.15	0.01	0.15
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	5	0.13	0.04	0.12
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	5	0.13	0.01	0.12
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	5	0.13	0.02	0.12
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	5	0.12	0.01	0.12
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	5	0.12	0.01	0.12
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	5	0.12	0.01	0.12
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	5	0.12	0.01	0.12
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	5	0.12	0.02	0.12
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	5	0.12	0.02	0.1
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	5	0.11	0.01	0.12
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	5	0.11	0.01	0.11
(1,1228)	1:197:A:ALA:HA	1:198:A:LEU:HD11	4	2.71	1.54	3.38
(1,295)	1:16:A:ILE:HG13	1:121:A:LEU:HD11	4	2.61	0.29	2.66
(1,1667)	1:54:A:SER:H	1:53:A:SER:HB3	4	1.4	0.01	1.4
(1,478)	1:47:A:LEU:HD11	1:84:A:ALA:HB1	4	1.38	0.29	1.35
(4,1)	1:74:A:LEU:HB3	1:106:A:GLN:HB2	4	1.17	0.5	1.16
(4,1)	1:78:A:LEU:HB3	1:112:A:ARG:HB2	4	1.17	0.5	1.16
(1,32)	1:6:A:MET:HA	1:9:A:LYS:HE2	4	0.84	0.41	0.76
(1,415)	1:36:A:LYS:HE3	1:188:A:PHE:HZ	4	0.8	0.22	0.8
(1,294)	1:16:A:ILE:HG12	1:121:A:LEU:HD11	4	0.78	0.35	0.76
(1,749)	1:103:A:GLU:HG3	1:105:A:GLN:HB3	4	0.6	0.13	0.54
(1,782)	1:112:A:ARG:HB2	1:113:A:ARG:HD2	4	0.53	0.21	0.5
(1,1774)	1:71:A:LEU:HD21	1:71:A:LEU:H	4	0.46	0.06	0.5
(1,1633)	1:48:A:LEU:H	1:47:A:LEU:HB2	4	0.4	0.47	0.16
(1,1867)	1:84:A:ALA:H	1:83:A:ASP:HB2	4	0.39	0.05	0.4
(1,341)	1:134:A:LEU:HD11	1:23:A:GLY:HA2	4	0.39	0.13	0.37
(1,888)	1:131:A:THR:HG21	1:132:A:GLN:HG2	4	0.37	0.27	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:71:A:LEU:HD21	1:71:A:LEU:HB3	4	0.29	0.02	0.29
(4,379)	1:37:A:TYR:H	1:36:A:LYS:HG2	4	0.22	0.11	0.18
(1,605)	1:78:A:LEU:HA	1:113:A:ARG:HD2	4	0.21	0.06	0.22
(1,77)	1:34:A:VAL:HG11	1:41:A:HIS:HB3	4	0.19	0.02	0.18
(1,77)	1:34:A:VAL:HG12	1:41:A:HIS:HB3	4	0.19	0.02	0.18
(1,1690)	1:58:A:ARG:H	1:58:A:ARG:HE	4	0.18	0.02	0.18
(1,1638)	1:49:A:ARG:H	1:46:A:ASP:HB2	4	0.17	0.04	0.18
(1,1770)	1:70:A:GLN:H	1:70:A:GLN:HG3	4	0.16	0.02	0.16
(1,1274)	1:61:A:LYS:H	1:61:A:LYS:HG3	4	0.14	0.03	0.14
(1,638)	1:84:A:ALA:HA	1:83:A:ASP:HB3	4	0.13	0.0	0.13
(1,1949)	1:95:A:PHE:H	1:15:A:ILE:HB	4	0.13	0.02	0.13
(1,2007)	1:104:A:VAL:H	1:105:A:GLN:H	4	0.13	0.02	0.13
(1,1517)	1:31:A:GLU:H	1:30:A:CYS:HB2	4	0.13	0.01	0.12
(4,364)	1:150:A:THR:H	1:151:A:ILE:HA	4	0.12	0.03	0.11
(1,2093)	1:119:A:LEU:H	1:15:A:ILE:HG21	4	0.12	0.02	0.11
(1,1435)	1:16:A:ILE:H	1:97:A:ILE:HB	4	0.11	0.02	0.11
(1,719)	1:97:A:ILE:HD11	1:97:A:ILE:HG21	4	0.11	0.01	0.11
(1,608)	1:78:A:LEU:HD11	1:74:A:LEU:HD21	3	2.03	1.36	2.97
(1,584)	1:74:A:LEU:HD11	1:106:A:GLN:HE22	3	1.87	1.24	2.72
(1,2566)	1:198:A:LEU:HD11	1:197:A:ALA:H	3	1.76	0.58	1.89
(1,2575)	1:199:A:LYS:H	1:198:A:LEU:HD11	3	1.69	0.28	1.86
(1,2572)	1:198:A:LEU:H	1:198:A:LEU:HD11	3	1.33	0.45	1.37
(1,412)	1:36:A:LYS:HE3	1:37:A:TYR:HD2	3	1.11	0.35	1.07
(1,73)	1:135:A:LEU:HD12	1:139:A:GLU:HG2	3	0.99	0.36	1.01
(1,73)	1:135:A:LEU:HD11	1:139:A:GLU:HG2	3	0.99	0.36	1.01
(1,73)	1:135:A:LEU:HD13	1:139:A:GLU:HG2	3	0.99	0.36	1.01
(1,1536)	1:34:A:VAL:H	1:35:A:GLN:HG2	3	0.89	0.02	0.89
(1,612)	1:78:A:LEU:HD21	1:106:A:GLN:HG3	3	0.79	0.45	0.61
(1,1379)	1:7:A:GLU:H	1:7:A:GLU:HB3	3	0.75	0.02	0.75
(1,610)	1:78:A:LEU:HD11	1:110:A:PHE:HD1	3	0.67	0.8	0.11
(4,340)	1:80:A:MET:H	1:76:A:THR:HG21	3	0.51	0.22	0.63
(4,340)	1:80:A:MET:H	1:76:A:THR:HG22	3	0.51	0.22	0.63
(4,151)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	3	0.42	0.0	0.42
(1,1605)	1:43:A:SER:H	1:42:A:LEU:HG	3	0.39	0.41	0.11
(1,1416)	1:14:A:LYS:H	1:14:A:LYS:HG2	3	0.31	0.14	0.24
(1,153)	1:166:A:ILE:HD12	1:162:A:THR:HG1	3	0.24	0.16	0.13
(1,1993)	1:102:A:ARG:H	1:102:A:ARG:HD2	3	0.22	0.05	0.22
(4,210)	1:170:A:GLU:HG2	1:170:A:GLU:HA	3	0.17	0.04	0.2
(4,305)	1:155:A:LEU:H	1:156:A:GLU:HG2	3	0.17	0.04	0.19
(4,359)	1:169:A:TYR:H	1:171:A:LYS:HB2	3	0.17	0.05	0.17
(1,587)	1:75:A:GLU:HA	1:74:A:LEU:HD11	3	0.16	0.02	0.15
(1,208)	1:152:A:LYS:HA	1:151:A:ILE:HG23	3	0.16	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2040)	1:108:A:GLU:H	1:106:A:GLN:HE21	3	0.15	0.02	0.14
(1,1652)	1:51:A:GLU:H	1:51:A:GLU:HG3	3	0.15	0.03	0.15
(1,1882)	1:85:A:MET:H	1:86:A:VAL:HG11	3	0.15	0.03	0.16
(1,1301)	1:83:A:ASP:H	1:83:A:ASP:HB2	3	0.15	0.03	0.16
(1,789)	1:114:A:ILE:HD11	1:79:A:ASP:HA	3	0.13	0.01	0.13
(1,1820)	1:79:A:ASP:H	1:77:A:VAL:HA	3	0.13	0.02	0.12
(1,2120)	1:122:A:TYR:H	1:122:A:TYR:HD1	3	0.13	0.03	0.11
(1,2289)	1:156:A:GLU:H	1:152:A:LYS:HD3	3	0.12	0.03	0.1
(1,462)	1:44:A:THR:HG21	1:48:A:LEU:HG	3	0.12	0.01	0.13
(1,1601)	1:42:A:LEU:H	1:96:A:LEU:HB2	3	0.12	0.01	0.12
(1,2082)	1:116:A:GLN:H	1:15:A:ILE:HG21	3	0.12	0.01	0.12
(1,1401)	1:12:A:LYS:H	1:11:A:LYS:HA	3	0.12	0.01	0.12
(1,273)	1:15:A:ILE:HD11	1:15:A:ILE:HG13	3	0.11	0.01	0.11
(1,1100)	1:168:A:PHE:HA	1:172:A:ARG:H	3	0.11	0.0	0.11
(1,1720)	1:63:A:SER:H	1:62:A:LEU:HB3	3	0.11	0.01	0.11
(1,928)	1:141:A:SER:HB3	1:141:A:SER:HA	3	0.11	0.01	0.11
(1,154)	1:76:A:THR:HB	1:48:A:LEU:HA	3	0.11	0.01	0.1
(1,795)	1:113:A:ARG:HG3	1:114:A:ILE:HD11	3	0.11	0.0	0.11
(1,1570)	1:39:A:TYR:H	1:37:A:TYR:HD1	3	0.11	0.0	0.11
(1,385)	1:195:A:LEU:HD21	1:33:A:ILE:HG21	3	0.1	0.0	0.1
(1,9)	1:74:A:LEU:HD12	1:73:A:PRO:HA	2	3.0	0.02	3.0
(1,581)	1:74:A:LEU:HD11	1:73:A:PRO:HD3	2	2.5	0.03	2.5
(4,68)	1:104:A:VAL:HG11	1:166:A:ILE:H	2	2.11	0.08	2.11
(1,525)	1:62:A:LEU:HD11	1:52:A:VAL:HG11	2	2.0	0.7	2.0
(1,109)	1:105:A:GLN:HA	1:104:A:VAL:HG23	2	1.98	0.02	1.98
(1,1184)	1:185:A:ASP:HA	1:184:A:VAL:HG21	2	1.94	0.01	1.94
(1,225)	1:6:A:MET:HB2	1:86:A:VAL:HG11	2	1.82	0.33	1.82
(1,258)	1:13:A:THR:HG21	1:10:A:LEU:HD11	2	1.7	0.55	1.7
(1,754)	1:104:A:VAL:HG11	1:164:A:PRO:HA	2	1.66	0.04	1.66
(1,1805)	1:76:A:THR:H	1:77:A:VAL:HG21	2	1.64	1.48	1.64
(1,250)	1:10:A:LEU:HD21	1:114:A:ILE:HG21	2	1.61	0.1	1.61
(1,361)	1:28:A:THR:HB	1:184:A:VAL:HG11	2	1.58	0.01	1.58
(1,1181)	1:183:A:SER:HA	1:184:A:VAL:HG11	2	1.5	0.02	1.5
(1,2336)	1:104:A:VAL:HG11	1:165:A:VAL:H	2	1.4	0.02	1.4
(1,1198)	1:187:A:VAL:HG21	1:191:A:VAL:HB	2	1.39	1.28	1.39
(4,84)	1:48:A:LEU:HD22	1:76:A:THR:HB	2	1.31	0.01	1.31
(4,84)	1:47:A:LEU:HD13	1:47:A:LEU:HA	2	1.31	0.01	1.31
(1,1259)	1:89:A:VAL:H	1:6:A:MET:HG2	2	1.3	0.2	1.3
(1,407)	1:36:A:LYS:HE2	1:36:A:LYS:HB3	2	1.17	0.04	1.17
(1,1353)	1:182:A:GLY:H	1:187:A:VAL:HG11	2	1.17	1.06	1.17
(1,1353)	1:182:A:GLY:H	1:187:A:VAL:HG13	2	1.17	1.06	1.17
(1,1182)	1:184:A:VAL:HG11	1:184:A:VAL:HA	2	1.16	0.01	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,752)	1:103:A:GLU:HA	1:104:A:VAL:HG11	2	1.04	0.01	1.04
(1,2005)	1:104:A:VAL:H	1:104:A:VAL:HG11	2	1.02	0.01	1.02
(1,7)	1:10:A:LEU:HD13	1:10:A:LEU:HB2	2	1.0	0.02	1.0
(1,760)	1:105:A:GLN:HA	1:104:A:VAL:HG21	2	0.98	0.04	0.98
(1,1515)	1:30:A:CYS:H	1:31:A:GLU:HG3	2	0.92	0.8	0.92
(1,30)	1:6:A:MET:HA	1:6:A:MET:HG2	2	0.89	0.01	0.89
(1,401)	1:35:A:GLN:HA	1:36:A:LYS:HB2	2	0.88	0.01	0.88
(1,902)	1:135:A:LEU:HB3	1:135:A:LEU:HD11	2	0.88	0.15	0.88
(1,889)	1:131:A:THR:HG21	1:135:A:LEU:HD11	2	0.86	0.72	0.86
(1,350)	1:26:A:LYS:HE3	1:22:A:PRO:HA	2	0.85	0.06	0.85
(1,2417)	1:176:A:ARG:H	1:177:A:LYS:HG3	2	0.78	0.66	0.78
(1,2486)	1:185:A:ASP:H	1:184:A:VAL:HG21	2	0.76	0.03	0.76
(1,248)	1:10:A:LEU:HD21	1:7:A:GLU:HG2	2	0.76	0.31	0.76
(1,2255)	1:150:A:THR:H	1:135:A:LEU:HD21	2	0.74	0.62	0.74
(1,680)	1:89:A:VAL:HG21	1:90:A:ASN:HD21	2	0.73	0.03	0.73
(1,598)	1:77:A:VAL:HG11	1:100:A:TYR:HE1	2	0.72	0.62	0.72
(1,582)	1:74:A:LEU:HD11	1:74:A:LEU:HA	2	0.69	0.03	0.69
(4,185)	1:198:A:LEU:HB3	1:198:A:LEU:HD22	2	0.64	0.03	0.64
(4,185)	1:135:A:LEU:HB3	1:135:A:LEU:HD12	2	0.64	0.03	0.64
(4,3)	1:10:A:LEU:HD13	1:13:A:THR:HA	2	0.6	0.34	0.6
(1,2481)	1:184:A:VAL:H	1:184:A:VAL:HG11	2	0.58	0.01	0.58
(1,2419)	1:177:A:LYS:H	1:176:A:ARG:HD2	2	0.58	0.1	0.58
(1,115)	1:104:A:VAL:HG23	1:105:A:GLN:HB2	2	0.56	0.04	0.56
(1,2218)	1:143:A:ARG:H	1:146:A:ASP:HB2	2	0.55	0.03	0.55
(1,249)	1:10:A:LEU:HD21	1:11:A:LYS:HD3	2	0.55	0.1	0.55
(1,2013)	1:105:A:GLN:H	1:104:A:VAL:HG21	2	0.54	0.0	0.54
(1,227)	1:7:A:GLU:HA	1:6:A:MET:HG2	2	0.45	0.04	0.45
(4,208)	1:156:A:GLU:HG3	1:157:A:THR:HG1	2	0.39	0.09	0.39
(1,653)	1:87:A:ALA:HB1	1:83:A:ASP:HB2	2	0.36	0.15	0.36
(4,112)	1:134:A:LEU:HD12	1:137:A:ARG:HD2	2	0.36	0.03	0.36
(4,112)	1:134:A:LEU:HD11	1:137:A:ARG:HD2	2	0.36	0.03	0.36
(1,1547)	1:36:A:LYS:H	1:36:A:LYS:HB2	2	0.36	0.01	0.36
(1,339)	1:23:A:GLY:HA3	1:134:A:LEU:HA	2	0.31	0.03	0.31
(1,1)	1:14:A:LYS:HG3	1:14:A:LYS:HA	2	0.3	0.12	0.3
(1,1790)	1:75:A:GLU:H	1:74:A:LEU:HD11	2	0.26	0.08	0.26
(1,2448)	1:180:A:ALA:H	1:124:A:ASP:HB2	2	0.25	0.11	0.25
(4,318)	1:65:A:ILE:H	1:62:A:LEU:HA	2	0.25	0.11	0.25
(1,343)	1:24:A:SER:HA	1:130:A:MET:HB2	2	0.23	0.03	0.23
(4,94)	1:76:A:THR:HG21	1:75:A:GLU:HB2	2	0.22	0.04	0.22
(1,1320)	1:12:A:LYS:H	1:12:A:LYS:HD2	2	0.19	0.07	0.19
(4,72)	1:103:A:GLU:HA	1:103:A:GLU:HG3	2	0.18	0.04	0.18
(4,72)	1:103:A:GLU:HA	1:164:A:PRO:HG2	2	0.18	0.04	0.18

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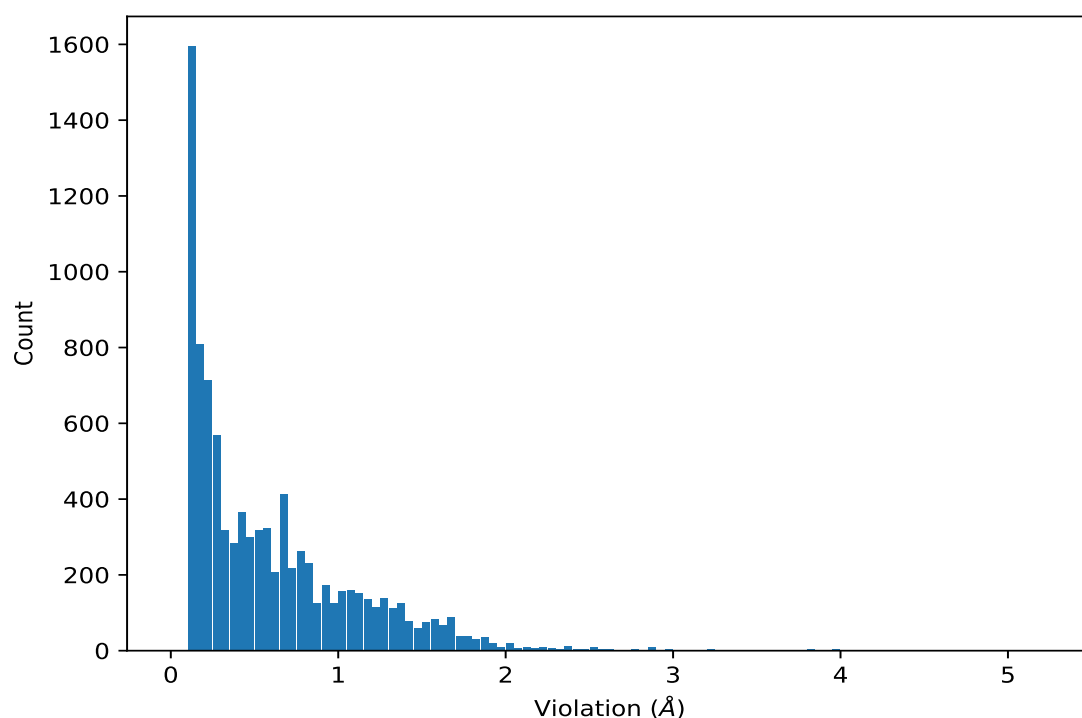
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,106)	1:184:A:VAL:HG22	1:188:A:PHE:H	2	0.18	0.0	0.18
(1,337)	1:23:A:GLY:HA2	1:133:A:ARG:HD3	2	0.18	0.06	0.18
(1,408)	1:36:A:LYS:HE3	1:36:A:LYS:HB3	2	0.18	0.02	0.18
(1,776)	1:111:A:GLU:HG3	1:116:A:GLN:HA	2	0.18	0.03	0.18
(1,2238)	1:146:A:ASP:H	1:147:A:ASN:HD22	2	0.18	0.03	0.18
(4,346)	1:90:A:ASN:H	1:86:A:VAL:HA	2	0.17	0.01	0.17
(1,108)	1:34:A:VAL:HG23	1:40:A:THR:HA	2	0.16	0.03	0.16
(1,331)	1:22:A:PRO:HA	1:26:A:LYS:HB2	2	0.16	0.06	0.16
(1,497)	1:57:A:ALA:HA	1:60:A:LYS:HE2	2	0.16	0.01	0.16
(1,758)	1:104:A:VAL:HG21	1:104:A:VAL:HB	2	0.15	0.0	0.15
(1,2426)	1:177:A:LYS:H	1:178:A:VAL:HG11	2	0.15	0.02	0.15
(1,296)	1:16:A:ILE:HA	1:16:A:ILE:HG21	2	0.14	0.01	0.14
(1,351)	1:26:A:LYS:HE2	1:26:A:LYS:HB2	2	0.14	0.01	0.14
(1,1543)	1:36:A:LYS:H	1:33:A:ILE:H	2	0.13	0.0	0.13
(1,121)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	2	0.12	0.02	0.12
(1,814)	1:118:A:THR:HG21	1:118:A:THR:HA	2	0.12	0.01	0.12
(1,2197)	1:139:A:GLU:H	1:139:A:GLU:HG2	2	0.12	0.02	0.12
(1,2300)	1:158:A:TYR:H	1:156:A:GLU:H	2	0.12	0.0	0.12
(4,116)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	2	0.12	0.0	0.12
(1,2023)	1:106:A:GLN:H	1:104:A:VAL:HA	2	0.11	0.01	0.11
(1,380)	1:33:A:ILE:HG21	1:37:A:TYR:HE1	2	0.11	0.0	0.11
(1,383)	1:33:A:ILE:HG21	1:39:A:TYR:HD1	2	0.11	0.0	0.11
(1,1553)	1:37:A:TYR:H	1:35:A:GLN:HB2	2	0.11	0.0	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)
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	5	5.21
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	10	4.13
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	12	3.98
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	14	3.97
(1,1228)	1:197:A:ALA:HA	1:198:A:LEU:HD11	6	3.96
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	14	3.86
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	4	3.82
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	2	3.82
(1,1228)	1:197:A:ALA:HA	1:198:A:LEU:HD11	19	3.81
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	2	3.79
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	10	3.75
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	12	3.71
(1,493)	1:52:A:VAL:HG11	1:62:A:LEU:HB2	3	3.55
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG21	14	3.51
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD11	9	3.38
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	14	3.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	16	3.31
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	15	3.3
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD11	13	3.25
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	4	3.23
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	9	3.21
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	2	3.2
(1,1805)	1:76:A:THR:H	1:77:A:VAL:HG21	5	3.12
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	5	3.1
(1,9)	1:74:A:LEU:HD12	1:73:A:PRO:HA	17	3.03
(1,608)	1:78:A:LEU:HD11	1:74:A:LEU:HD21	11	3.01
(1,9)	1:74:A:LEU:HD12	1:73:A:PRO:HA	11	2.98
(1,608)	1:78:A:LEU:HD11	1:74:A:LEU:HD21	17	2.97
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	18	2.97
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD11	1	2.95
(1,1228)	1:197:A:ALA:HA	1:198:A:LEU:HD11	15	2.95
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	5	2.94
(1,97)	1:52:A:VAL:HG13	1:58:A:ARG:HD2	3	2.91
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	1	2.9
(1,295)	1:16:A:ILE:HG13	1:121:A:LEU:HD11	18	2.9
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	14	2.89
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	19	2.89
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	18	2.88
(1,494)	1:52:A:VAL:HG21	1:53:A:SER:HA	3	2.88
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	20	2.88
(1,325)	1:19:A:VAL:HG11	1:120:A:LEU:HD11	19	2.87
(1,295)	1:16:A:ILE:HG13	1:121:A:LEU:HD11	6	2.87
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	6	2.8
(1,584)	1:74:A:LEU:HD11	1:106:A:GLN:HE22	11	2.78
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	10	2.78
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	16	2.75
(1,584)	1:74:A:LEU:HD11	1:106:A:GLN:HE22	17	2.72
(1,525)	1:62:A:LEU:HD11	1:52:A:VAL:HG11	3	2.71
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	18	2.69
(1,1198)	1:187:A:VAL:HG21	1:191:A:VAL:HB	14	2.67
(1,938)	1:144:A:VAL:HG21	1:143:A:ARG:HA	16	2.65
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	2	2.62
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	15	2.61
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	16	2.6
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	10	2.6
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	3	2.59
(1,527)	1:59:A:GLY:HA3	1:62:A:LEU:HD11	4	2.59
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	13	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	1	2.57
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	11	2.57
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	17	2.55
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	15	2.53
(1,603)	1:77:A:VAL:HG11	1:78:A:LEU:HA	5	2.53
(1,581)	1:74:A:LEU:HD11	1:73:A:PRO:HD3	17	2.53
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	13	2.51
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	6	2.51
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	9	2.51
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	18	2.5
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	10	2.49
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	9	2.49
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	4	2.47
(1,581)	1:74:A:LEU:HD11	1:73:A:PRO:HD3	11	2.46
(1,295)	1:16:A:ILE:HG13	1:121:A:LEU:HD11	20	2.46
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	1	2.44
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	1	2.43
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	13	2.42
(1,2566)	1:198:A:LEU:HD11	1:197:A:ALA:H	6	2.4
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	20	2.4
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	20	2.39
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	4	2.39
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	3	2.38
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	7	2.37
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	9	2.37
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	19	2.35
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	18	2.35
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	10	2.35
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	6	2.35
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	16	2.32
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	12	2.31
(1,904)	1:135:A:LEU:HD11	1:136:A:LYS:HD2	9	2.31
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	16	2.31
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	2	2.31
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	17	2.3
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	19	2.3
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	5	2.29
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	7	2.28
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	8	2.27
(1,258)	1:13:A:THR:HG21	1:10:A:LEU:HD11	2	2.26
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	20	2.25
(1,1353)	1:182:A:GLY:H	1:187:A:VAL:HG13	14	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	11	2.23
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	17	2.23
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	6	2.22
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	17	2.22
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	4	2.21
(1,295)	1:16:A:ILE:HG13	1:121:A:LEU:HD11	11	2.21
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	14	2.2
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	19	2.2
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	20	2.2
(4,68)	1:104:A:VAL:HG11	1:166:A:ILE:H	15	2.19
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	7	2.19
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	16	2.19
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	8	2.17
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	14	2.16
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	12	2.16
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	16	2.15
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD23	6	2.14
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	12	2.14
(1,225)	1:6:A:MET:HB2	1:86:A:VAL:HG11	12	2.14
(1,1961)	1:96:A:LEU:H	1:96:A:LEU:HD11	1	2.13
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	1	2.13
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	3	2.13
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	5	2.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	6	2.12
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	10	2.12
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	2	2.11
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	19	2.09
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	3	2.09
(1,1197)	1:187:A:VAL:HG21	1:190:A:GLN:HG2	14	2.08
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	14	2.06
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	16	2.06
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	9	2.06
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	11	2.05
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	17	2.05
(4,20)	1:74:A:LEU:HG	1:105:A:GLN:HB2	11	2.05
(4,20)	1:74:A:LEU:HG	1:105:A:GLN:HB2	17	2.05
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	6	2.05
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	6	2.05
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	15	2.05
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	12	2.04
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	14	2.04
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	17	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD23	19	2.03
(4,68)	1:104:A:VAL:HG11	1:166:A:ILE:H	3	2.03
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	4	2.03
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	1	2.02
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	18	2.02
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD22	18	2.01
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	9	2.01
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	6	2.0
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	8	2.0
(1,109)	1:105:A:GLN:HA	1:104:A:VAL:HG23	3	2.0
(1,495)	1:52:A:VAL:HG21	1:53:A:SER:HB2	3	1.98
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	6	1.98
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	18	1.97
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	9	1.97
(1,109)	1:105:A:GLN:HA	1:104:A:VAL:HG23	15	1.97
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	17	1.97
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	19	1.96
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	2	1.96
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	7	1.96
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	11	1.95
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	12	1.95
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	16	1.94
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	20	1.94
(1,1184)	1:185:A:ASP:HA	1:184:A:VAL:HG21	14	1.94
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	19	1.94
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	12	1.94
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	20	1.93
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	15	1.93
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	10	1.93
(1,1184)	1:185:A:ASP:HA	1:184:A:VAL:HG21	10	1.93
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	20	1.93
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	10	1.93
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	13	1.92
(1,2575)	1:199:A:LYS:H	1:198:A:LEU:HD11	19	1.92
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	17	1.92
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	20	1.92
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD23	16	1.91
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	11	1.91
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	10	1.91
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	8	1.9
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	12	1.9
(4,147)	1:197:A:ALA:HB1	1:121:A:LEU:HD21	13	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	5	1.9
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	9	1.9
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	1	1.89
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	6	1.89
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	12	1.89
(1,2566)	1:198:A:LEU:HD11	1:197:A:ALA:H	19	1.89
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	4	1.89
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	14	1.89
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	20	1.89
(4,169)	1:65:A:ILE:HD11	1:48:A:LEU:HB3	9	1.88
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	13	1.88
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	14	1.88
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	20	1.88
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	15	1.88
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	18	1.88
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	12	1.88
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	3	1.87
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	16	1.87
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	9	1.87
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	10	1.87
(1,2047)	1:110:A:PHE:H	1:78:A:LEU:HD11	16	1.87
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	2	1.87
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	4	1.86
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	17	1.86
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	1	1.86
(4,1)	1:78:A:LEU:HB3	1:112:A:ARG:HB2	2	1.86
(1,2575)	1:199:A:LYS:H	1:198:A:LEU:HD11	6	1.86
(1,2572)	1:198:A:LEU:H	1:198:A:LEU:HD11	6	1.86
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	14	1.85
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	19	1.85
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	1	1.85
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	5	1.85
(4,147)	1:197:A:ALA:HB1	1:121:A:LEU:HD21	20	1.84
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	13	1.84
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	3	1.84
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	17	1.84
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	20	1.84
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	7	1.84
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	11	1.84
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	15	1.83
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	7	1.83
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	15	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,147)	1:84:A:ALA:HB1	1:15:A:ILE:HD12	3	1.83
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	18	1.83
(4,217)	1:43:A:SER:HB3	1:42:A:LEU:HD12	20	1.82
(4,169)	1:65:A:ILE:HD13	1:48:A:LEU:HB3	13	1.82
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	1	1.82
(4,10)	1:71:A:LEU:HG	1:65:A:ILE:HG23	14	1.82
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	13	1.82
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	4	1.82
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	6	1.82
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	4	1.82
(1,478)	1:47:A:LEU:HD11	1:84:A:ALA:HB1	20	1.82
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	8	1.81
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	16	1.81
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	8	1.81
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	5	1.8
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	5	1.8
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	4	1.8
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	3	1.8
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	5	1.8
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	17	1.8
(1,610)	1:78:A:LEU:HD11	1:110:A:PHE:HD1	16	1.8
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	8	1.79
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	15	1.79
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	5	1.79
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	5	1.79
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	10	1.79
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	13	1.79
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	12	1.79
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	15	1.79
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	5	1.78
(1,1698)	1:59:A:GLY:H	1:62:A:LEU:HD11	4	1.78
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	15	1.78
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	14	1.78
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	10	1.77
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	14	1.77
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	19	1.77
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	4	1.77
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	9	1.77
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	16	1.77
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	17	1.77
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	2	1.77
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	10	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	1	1.77
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	6	1.76
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG23	15	1.76
(1,2225)	1:144:A:VAL:H	1:144:A:VAL:HG21	16	1.76
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	11	1.76
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	12	1.76
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	18	1.76
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	16	1.76
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	7	1.76
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	17	1.76
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	2	1.76
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	7	1.75
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	8	1.75
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	2	1.75
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	16	1.75
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	17	1.75
(4,194)	1:65:A:ILE:HB	1:62:A:LEU:HD13	2	1.74
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	20	1.74
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	20	1.74
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	1	1.74
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	19	1.74
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	3	1.74
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	19	1.74
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	7	1.74
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	11	1.73
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	7	1.73
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	7	1.73
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	6	1.73
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	12	1.73
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	20	1.73
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	5	1.72
(4,123)	1:144:A:VAL:HG12	1:22:A:PRO:HD2	2	1.72
(1,1515)	1:30:A:CYS:H	1:31:A:GLU:HG3	14	1.72
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	4	1.72
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	5	1.72
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	16	1.72
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	14	1.72
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	20	1.72
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	2	1.72
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	13	1.72
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	1	1.72
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	14	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	2	1.72
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	13	1.72
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	20	1.72
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	4	1.72
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	14	1.71
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	5	1.71
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	17	1.71
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	18	1.71
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	6	1.71
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	2	1.71
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	6	1.71
(1,250)	1:10:A:LEU:HD21	1:114:A:ILE:HG21	12	1.71
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	2	1.7
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	3	1.7
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	11	1.7
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	20	1.7
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	4	1.7
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	13	1.7
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	1	1.7
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	19	1.7
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	3	1.7
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	5	1.7
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	8	1.7
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	12	1.7
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	11	1.7
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	19	1.7
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	2	1.7
(1,983)	1:151:A:ILE:HD11	1:154:A:ARG:HH21	14	1.7
(1,905)	1:135:A:LEU:HD11	1:136:A:LYS:HE3	9	1.7
(1,754)	1:104:A:VAL:HG11	1:164:A:PRO:HA	3	1.7
(1,472)	1:47:A:LEU:HD11	1:47:A:LEU:HA	20	1.7
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	6	1.7
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	19	1.7
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	3	1.7
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	5	1.7
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	11	1.7
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	16	1.7
(1,308)	1:18:A:VAL:HA	1:120:A:LEU:HD11	19	1.7
(4,288)	1:93:A:LYS:H	1:16:A:ILE:HG13	20	1.69
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	9	1.69
(4,147)	1:84:A:ALA:HB1	1:15:A:ILE:HD12	11	1.69
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	13	1.69
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	2	1.69
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	13	1.69
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	12	1.69
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	13	1.69
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	4	1.69
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	9	1.69
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	18	1.69
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	1	1.69
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	3	1.69
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	10	1.69
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	7	1.69
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	10	1.69
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	1	1.69
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	5	1.69
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	5	1.69
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	11	1.69
(4,199)	1:156:A:GLU:HG3	1:152:A:LYS:HD2	20	1.68
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HB2	10	1.68
(4,160)	1:97:A:ILE:HG21	1:77:A:VAL:HA	18	1.68
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	7	1.68
(1,2320)	1:161:A:ALA:H	1:160:A:LYS:HD3	12	1.68
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	10	1.68
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	11	1.68
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	15	1.68
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	7	1.68
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	14	1.68
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	9	1.68
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	20	1.68
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	15	1.68
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	9	1.68
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	12	1.68
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	14	1.68
(4,160)	1:97:A:ILE:HG21	1:110:A:PHE:HB2	19	1.67
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	12	1.67
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	9	1.67
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	18	1.67
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	10	1.67
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	10	1.67
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	16	1.67
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	4	1.67
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	7	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	15	1.67
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	17	1.67
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	14	1.66
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	16	1.66
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	19	1.66
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	9	1.66
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	16	1.66
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	20	1.66
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	2	1.66
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	15	1.66
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	18	1.66
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	18	1.66
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	4	1.66
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	17	1.66
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	20	1.66
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	12	1.66
(4,288)	1:93:A:LYS:H	1:16:A:ILE:HG13	17	1.65
(4,198)	1:77:A:VAL:HA	1:47:A:LEU:HB2	2	1.65
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	8	1.65
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	3	1.65
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	16	1.65
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	20	1.65
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	11	1.65
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	5	1.65
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	3	1.65
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	12	1.65
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	17	1.65
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	20	1.65
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	10	1.65
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	5	1.65
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	10	1.64
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	15	1.64
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	16	1.64
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	14	1.64
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	18	1.64
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	7	1.64
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	12	1.63
(4,288)	1:93:A:LYS:H	1:16:A:ILE:HG13	16	1.63
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	19	1.63
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	1	1.63
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	9	1.63
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	20	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	19	1.63
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	1	1.63
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	8	1.63
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	10	1.63
(4,123)	1:144:A:VAL:HG12	1:22:A:PRO:HD2	10	1.62
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	14	1.62
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	11	1.62
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	16	1.62
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	4	1.62
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	10	1.62
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	17	1.62
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	7	1.62
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	17	1.62
(1,754)	1:104:A:VAL:HG11	1:164:A:PRO:HA	15	1.62
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	16	1.62
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	7	1.62
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	11	1.62
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	18	1.62
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	1	1.62
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	14	1.62
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	3	1.62
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	10	1.62
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	6	1.61
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	14	1.61
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	15	1.61
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	8	1.61
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	17	1.61
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	16	1.61
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	8	1.6
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	18	1.6
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	14	1.6
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	7	1.6
(1,2234)	1:146:A:ASP:H	1:144:A:VAL:HG21	16	1.6
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	8	1.6
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	2	1.6
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	12	1.6
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	2	1.6
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	6	1.6
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	15	1.6
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	2	1.6
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	10	1.6
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	4	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	12	1.59
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HB2	17	1.59
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	5	1.59
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	14	1.59
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	18	1.59
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	9	1.59
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	13	1.59
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	15	1.59
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	14	1.59
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	4	1.59
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	6	1.59
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	13	1.59
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	8	1.59
(1,361)	1:28:A:THR:HB	1:184:A:VAL:HG11	10	1.59
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	9	1.58
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	13	1.58
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HB2	20	1.58
(4,140)	1:89:A:VAL:HG21	1:86:A:VAL:HG21	13	1.58
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	13	1.58
(4,76)	1:104:A:VAL:HG12	1:166:A:ILE:HA	2	1.58
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	17	1.58
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	2	1.58
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	13	1.58
(1,988)	1:151:A:ILE:HG21	1:135:A:LEU:HG	9	1.58
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	5	1.58
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	16	1.58
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	11	1.58
(1,889)	1:131:A:THR:HG21	1:135:A:LEU:HD11	9	1.58
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	4	1.58
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	5	1.58
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	15	1.58
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	19	1.58
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	13	1.58
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	20	1.58
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	11	1.57
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	2	1.57
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	4	1.57
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	9	1.57
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	20	1.57
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	10	1.57
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	19	1.57
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	5	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	12	1.57
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	9	1.57
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	12	1.57
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	1	1.57
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	8	1.57
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	11	1.57
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	3	1.57
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	14	1.57
(1,361)	1:28:A:THR:HB	1:184:A:VAL:HG11	14	1.57
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	1	1.57
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	7	1.56
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	10	1.56
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	6	1.56
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	11	1.56
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	20	1.56
(1,1716)	1:63:A:SER:H	1:52:A:VAL:HG11	3	1.56
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	19	1.56
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	4	1.56
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	6	1.56
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	1	1.56
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	8	1.56
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	12	1.56
(1,412)	1:36:A:LYS:HE3	1:37:A:TYR:HD2	6	1.56
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	11	1.56
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	12	1.56
(4,76)	1:10:A:LEU:HD22	1:86:A:VAL:HA	18	1.55
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	3	1.55
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	11	1.55
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	15	1.55
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	1	1.55
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	2	1.55
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	3	1.55
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	6	1.55
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	19	1.55
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	14	1.55
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	9	1.55
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	16	1.55
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	4	1.55
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	1	1.55
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	8	1.55
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	19	1.55
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	14	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	5	1.54
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	19	1.54
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	8	1.54
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	3	1.54
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	14	1.54
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	15	1.54
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	16	1.54
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	17	1.54
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	4	1.54
(1,359)	1:28:A:THR:HA	1:31:A:GLU:HB3	8	1.54
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	17	1.54
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	8	1.54
(4,288)	1:93:A:LYS:H	1:16:A:ILE:HG13	1	1.53
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	5	1.53
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	9	1.53
(4,123)	1:144:A:VAL:HG12	1:22:A:PRO:HD2	14	1.53
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	9	1.53
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	14	1.53
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	6	1.53
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	1	1.53
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	2	1.53
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	13	1.53
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	6	1.53
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	7	1.53
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	20	1.53
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	11	1.53
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	7	1.53
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	14	1.53
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	16	1.52
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	4	1.52
(4,147)	1:197:A:ALA:HB1	1:121:A:LEU:HD21	16	1.52
(4,140)	1:34:A:VAL:HG22	1:33:A:ILE:HG22	1	1.52
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	1	1.52
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	2	1.52
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	5	1.52
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	11	1.52
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	16	1.52
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	15	1.52
(1,1181)	1:183:A:SER:HA	1:184:A:VAL:HG11	10	1.52
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	7	1.52
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	2	1.52
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	4	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:86:A:VAL:HG11	1:6:A:MET:HG3	12	1.52
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	4	1.52
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	9	1.52
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	15	1.52
(4,143)	1:89:A:VAL:HG22	1:88:A:LYS:HD2	16	1.51
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	4	1.51
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	7	1.51
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	10	1.51
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	20	1.51
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	11	1.51
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	19	1.51
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	5	1.51
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	6	1.51
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	12	1.51
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	19	1.51
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	4	1.51
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	2	1.51
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	3	1.51
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	20	1.51
(1,250)	1:10:A:LEU:HD21	1:114:A:ILE:HG21	2	1.51
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	4	1.51
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	3	1.5
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	12	1.5
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	5	1.5
(1,1259)	1:89:A:VAL:H	1:6:A:MET:HG2	12	1.5
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	6	1.5
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	10	1.5
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	8	1.5
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	19	1.5
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	20	1.5
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	5	1.5
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	13	1.5
(1,54)	1:184:A:VAL:HA	1:187:A:VAL:HG13	14	1.5
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	8	1.49
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	13	1.49
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	17	1.49
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	18	1.49
(1,2064)	1:113:A:ARG:H	1:109:A:GLU:HG2	2	1.49
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	10	1.49
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	20	1.49
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	6	1.49
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	7	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	7	1.49
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	16	1.49
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	9	1.49
(1,225)	1:6:A:MET:HB2	1:86:A:VAL:HG11	10	1.49
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	9	1.48
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	1	1.48
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	13	1.48
(1,1181)	1:183:A:SER:HA	1:184:A:VAL:HG11	14	1.48
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	1	1.48
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	3	1.48
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	18	1.48
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	10	1.48
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	9	1.48
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	18	1.48
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	19	1.48
(1,32)	1:6:A:MET:HA	1:9:A:LYS:HE2	16	1.48
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	6	1.47
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	1	1.47
(4,198)	1:77:A:VAL:HA	1:47:A:LEU:HB2	8	1.47
(4,123)	1:144:A:VAL:HG11	1:22:A:PRO:HD2	7	1.47
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	10	1.47
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	16	1.47
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	15	1.47
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	8	1.47
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	9	1.47
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	19	1.47
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	11	1.47
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	13	1.47
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	16	1.47
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	8	1.47
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	20	1.47
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	12	1.47
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	13	1.47
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	1	1.47
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	4	1.47
(1,502)	1:57:A:ALA:HB1	1:60:A:LYS:HD3	19	1.47
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	14	1.47
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	6	1.46
(4,123)	1:144:A:VAL:HG11	1:22:A:PRO:HD2	20	1.46
(4,107)	1:129:A:THR:HG21	1:128:A:GLU:HG3	17	1.46
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	19	1.46
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	11	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	14	1.46
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	12	1.46
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	2	1.46
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	12	1.46
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	8	1.46
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	15	1.46
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	18	1.46
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	2	1.46
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	11	1.46
(4,198)	1:77:A:VAL:HA	1:47:A:LEU:HB2	3	1.45
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	14	1.45
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	17	1.45
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	19	1.45
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD13	2	1.45
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	4	1.45
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	4	1.45
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	5	1.45
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	13	1.45
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	18	1.45
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	1	1.45
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	18	1.45
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	5	1.45
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	3	1.45
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	19	1.45
(4,204)	1:28:A:THR:HA	1:29:A:GLN:HB3	4	1.44
(4,204)	1:28:A:THR:HA	1:29:A:GLN:HB3	11	1.44
(1,2417)	1:176:A:ARG:H	1:177:A:LYS:HG3	8	1.44
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	18	1.44
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	3	1.44
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	6	1.44
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	1	1.44
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	20	1.44
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	18	1.44
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	11	1.44
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	7	1.44
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	13	1.44
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	9	1.44
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	8	1.44
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	4	1.44
(4,288)	1:93:A:LYS:H	1:42:A:LEU:HD11	15	1.43
(4,204)	1:28:A:THR:HA	1:29:A:GLN:HB3	18	1.43
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	11	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	7	1.43
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	10	1.43
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	16	1.43
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	14	1.43
(4,204)	1:28:A:THR:HA	1:29:A:GLN:HB3	17	1.42
(4,169)	1:65:A:ILE:HD11	1:48:A:LEU:HB3	8	1.42
(1,2336)	1:104:A:VAL:HG11	1:165:A:VAL:H	15	1.42
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	3	1.42
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	6	1.42
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	16	1.42
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	15	1.42
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	14	1.42
(1,1495)	1:25:A:GLY:H	1:26:A:LYS:HG3	5	1.42
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	11	1.42
(1,781)	1:113:A:ARG:HD2	1:109:A:GLU:HB2	20	1.42
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	1	1.42
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	10	1.42
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	1	1.42
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	13	1.42
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	20	1.42
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	1	1.42
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	7	1.42
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	9	1.42
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	18	1.42
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	19	1.42
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	20	1.42
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	15	1.42
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	14	1.42
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	20	1.42
(4,147)	1:197:A:ALA:HB1	1:16:A:ILE:HD13	18	1.41
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	6	1.41
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	5	1.41
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	7	1.41
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	8	1.41
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	2	1.41
(1,1667)	1:54:A:SER:H	1:53:A:SER:HB3	17	1.41
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	19	1.41
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	8	1.41
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	6	1.41
(1,612)	1:78:A:LEU:HD21	1:106:A:GLN:HG3	16	1.41
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	3	1.41
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	5	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	13	1.41
(1,73)	1:135:A:LEU:HD11	1:139:A:GLU:HG2	19	1.41
(4,126)	1:144:A:VAL:HG12	1:154:A:ARG:HB3	15	1.4
(4,76)	1:10:A:LEU:HD22	1:86:A:VAL:HA	19	1.4
(1,2565)	1:197:A:ALA:H	1:198:A:LEU:HB2	15	1.4
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	10	1.4
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	13	1.4
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	15	1.4
(1,1667)	1:54:A:SER:H	1:53:A:SER:HB3	5	1.4
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	3	1.4
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	14	1.4
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	18	1.4
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	19	1.4
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	15	1.4
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	1	1.4
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	8	1.39
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	12	1.39
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	2	1.39
(1,1667)	1:54:A:SER:H	1:53:A:SER:HB3	9	1.39
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	19	1.39
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	19	1.39
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	10	1.39
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	20	1.39
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	18	1.39
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	11	1.39
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	20	1.39
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	19	1.39
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	11	1.39
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	14	1.39
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	6	1.39
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	13	1.39
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	15	1.39
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	18	1.38
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	20	1.38
(1,2336)	1:104:A:VAL:HG11	1:165:A:VAL:H	3	1.38
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	7	1.38
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	9	1.38
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	16	1.38
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	20	1.38
(1,1667)	1:54:A:SER:H	1:53:A:SER:HB3	13	1.38
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	18	1.38
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	2	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	8	1.38
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	12	1.38
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	5	1.38
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	6	1.38
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	12	1.38
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	7	1.38
(1,478)	1:47:A:LEU:HD11	1:84:A:ALA:HB1	6	1.38
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	13	1.38
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	9	1.38
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	10	1.38
(1,81)	1:76:A:THR:HG23	1:58:A:ARG:HD2	12	1.38
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	1	1.38
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	5	1.38
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	14	1.37
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	17	1.37
(4,1)	1:74:A:LEU:HB3	1:106:A:GLN:HB2	16	1.37
(1,2572)	1:198:A:LEU:H	1:198:A:LEU:HD11	19	1.37
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	9	1.37
(1,2288)	1:155:A:LEU:H	1:155:A:LEU:HD21	4	1.37
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	2	1.37
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	10	1.37
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	16	1.37
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	8	1.37
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	5	1.37
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	12	1.37
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	16	1.37
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	11	1.37
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	17	1.37
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	4	1.37
(1,526)	1:62:A:LEU:HD11	1:58:A:ARG:HG2	7	1.37
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	17	1.37
(1,363)	1:28:A:THR:HG21	1:29:A:GLN:HG3	16	1.37
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	11	1.37
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	4	1.37
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	5	1.37
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	1	1.36
(4,123)	1:144:A:VAL:HG12	1:22:A:PRO:HD2	6	1.36
(4,123)	1:144:A:VAL:HG13	1:22:A:PRO:HD2	9	1.36
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	11	1.36
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	20	1.36
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	18	1.36
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	15	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	1	1.36
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	4	1.36
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	9	1.36
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	17	1.36
(1,599)	1:77:A:VAL:HG21	1:73:A:PRO:HD3	1	1.36
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	8	1.36
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	10	1.36
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	18	1.36
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	12	1.36
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	19	1.36
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	3	1.36
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	12	1.36
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	17	1.35
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	18	1.35
(4,204)	1:157:A:THR:HA	1:160:A:LYS:HB3	9	1.35
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	3	1.35
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	3	1.35
(4,108)	1:178:A:VAL:HG12	1:190:A:GLN:HG3	18	1.35
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	15	1.35
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	8	1.35
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	9	1.35
(1,2255)	1:150:A:THR:H	1:135:A:LEU:HD21	9	1.35
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	4	1.35
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	6	1.35
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	13	1.35
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	15	1.35
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	19	1.35
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	13	1.35
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	11	1.35
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	18	1.35
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	1	1.35
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	10	1.35
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	16	1.35
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	15	1.35
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	6	1.35
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	18	1.35
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	7	1.35
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	19	1.35
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	3	1.35
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	5	1.35
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	6	1.35
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	8	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	7	1.35
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	12	1.35
(4,367)	1:13:A:THR:H	1:11:A:LYS:HG2	2	1.34
(4,335)	1:83:A:ASP:H	1:86:A:VAL:HG21	4	1.34
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	17	1.34
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	19	1.34
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	5	1.34
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	17	1.34
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	13	1.34
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	15	1.34
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	5	1.34
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	12	1.34
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	6	1.34
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	10	1.34
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	17	1.34
(1,598)	1:77:A:VAL:HG11	1:100:A:TYR:HE1	5	1.34
(1,580)	1:73:A:PRO:HD3	1:76:A:THR:HB	5	1.34
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	10	1.34
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	2	1.34
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	4	1.33
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	10	1.33
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	19	1.33
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD1	16	1.33
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	3	1.33
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	19	1.33
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	15	1.33
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	8	1.33
(1,1528)	1:32:A:LYS:H	1:33:A:ILE:HG13	9	1.33
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	18	1.33
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	15	1.33
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	16	1.33
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	17	1.33
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	11	1.33
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	3	1.33
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	3	1.33
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	16	1.33
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	14	1.33
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	17	1.33
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	6	1.33
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	19	1.32
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	5	1.32
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD1	12	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD1	17	1.32
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	4	1.32
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	4	1.32
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	11	1.32
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	19	1.32
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	20	1.32
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	7	1.32
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	8	1.32
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	16	1.32
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	2	1.32
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	15	1.32
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	10	1.32
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	14	1.32
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	13	1.32
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	9	1.32
(1,685)	1:90:A:ASN:HB2	1:91:A:THR:HG21	5	1.32
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	8	1.32
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	9	1.32
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	5	1.32
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	6	1.32
(1,478)	1:47:A:LEU:HD11	1:84:A:ALA:HB1	17	1.32
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	17	1.32
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	2	1.32
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	5	1.31
(4,84)	1:47:A:LEU:HD13	1:47:A:LEU:HA	5	1.31
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	8	1.31
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	16	1.31
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	14	1.31
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	5	1.31
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	7	1.31
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	14	1.31
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	1	1.31
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	2	1.31
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	4	1.31
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	5	1.31
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	12	1.31
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	2	1.31
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	7	1.31
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	18	1.31
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	3	1.31
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	14	1.31
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	7	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	12	1.31
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	1	1.31
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	1	1.31
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	9	1.31
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	1	1.3
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	2	1.3
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	20	1.3
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	14	1.3
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	8	1.3
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	20	1.3
(4,84)	1:48:A:LEU:HD22	1:76:A:THR:HB	2	1.3
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	18	1.3
(4,76)	1:104:A:VAL:HG11	1:160:A:LYS:HE3	7	1.3
(1,2575)	1:199:A:LYS:H	1:198:A:LEU:HD11	15	1.3
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	18	1.3
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	2	1.3
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	7	1.3
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	1	1.3
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	10	1.3
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	16	1.3
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	18	1.3
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	5	1.3
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	1	1.3
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	16	1.3
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	20	1.3
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	19	1.3
(1,525)	1:62:A:LEU:HD11	1:52:A:VAL:HG11	4	1.3
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	18	1.3
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	1	1.3
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	4	1.3
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	17	1.3
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	13	1.29
(4,217)	1:47:A:LEU:HD13	1:43:A:SER:HB3	2	1.29
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	13	1.29
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	1	1.29
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	12	1.29
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	2	1.29
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	12	1.29
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	15	1.29
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	18	1.29
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	6	1.29
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	3	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	6	1.29
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	6	1.29
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	7	1.29
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	13	1.29
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	19	1.29
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	3	1.29
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	14	1.28
(4,169)	1:65:A:ILE:HD11	1:68:A:LYS:HD2	1	1.28
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	13	1.28
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	16	1.28
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	2	1.28
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	6	1.28
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	8	1.28
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	17	1.28
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	17	1.28
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	10	1.28
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	13	1.28
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	19	1.28
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	12	1.28
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	18	1.28
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	9	1.28
(1,1284)	1:152:A:LYS:H	1:152:A:LYS:HE3	20	1.28
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	1	1.28
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	19	1.28
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	5	1.28
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	18	1.28
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	7	1.28
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	6	1.28
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	14	1.28
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	11	1.28
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	11	1.28
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	16	1.27
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	11	1.27
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	19	1.27
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	4	1.27
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	15	1.27
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	14	1.27
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	5	1.27
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	12	1.27
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	15	1.27
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	18	1.27
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	9	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	5	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	2	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	3	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	5	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	10	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	11	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	12	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	13	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	15	1.27
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	19	1.27
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	20	1.27
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	10	1.27
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	16	1.27
(1,702)	1:96:A:LEU:HB2	1:96:A:LEU:HD11	1	1.27
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	13	1.27
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	1	1.27
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	16	1.27
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	17	1.27
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	2	1.27
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	4	1.27
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	11	1.27
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	14	1.27
(1,367)	1:31:A:GLU:HG3	1:30:A:CYS:HB2	5	1.27
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	10	1.27
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	13	1.27
(4,107)	1:44:A:THR:HG22	1:77:A:VAL:HB	9	1.26
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	9	1.26
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	2	1.26
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	16	1.26
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	10	1.26
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	3	1.26
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	5	1.26
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	12	1.26
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	14	1.26
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	1	1.26
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	8	1.26
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	9	1.26
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	17	1.26
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	14	1.26
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	7	1.26
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	9	1.26
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	13	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	20	1.26
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	18	1.26
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	13	1.26
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	8	1.26
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	7	1.26
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	13	1.26
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	10	1.26
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	15	1.26
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	14	1.26
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	6	1.26
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	16	1.26
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	3	1.26
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	14	1.25
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	20	1.25
(4,169)	1:65:A:ILE:HD12	1:48:A:LEU:HB3	5	1.25
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	1	1.25
(4,147)	1:84:A:ALA:HB3	1:15:A:ILE:HD12	2	1.25
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	10	1.25
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	11	1.25
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	16	1.25
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	19	1.25
(1,2319)	1:161:A:ALA:H	1:160:A:LYS:HB2	19	1.25
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	16	1.25
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	14	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	2	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	6	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	7	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	8	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	16	1.25
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	17	1.25
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	17	1.25
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	14	1.25
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	4	1.25
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	14	1.25
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	19	1.25
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	4	1.25
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	1	1.25
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	18	1.25
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	6	1.25
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	20	1.25
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	12	1.25
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	18	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	12	1.25
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	12	1.25
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	16	1.24
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	6	1.24
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	7	1.24
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	13	1.24
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	2	1.24
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	1	1.24
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	11	1.24
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	13	1.24
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	20	1.24
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	5	1.24
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	20	1.24
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	10	1.24
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	8	1.24
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	19	1.24
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	4	1.24
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	17	1.24
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	7	1.24
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	13	1.24
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	19	1.24
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	8	1.24
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	12	1.24
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	20	1.24
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	1	1.24
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	5	1.24
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	5	1.24
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	12	1.23
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	2	1.23
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	4	1.23
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	19	1.23
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	11	1.23
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	18	1.23
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	6	1.23
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	2	1.23
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	19	1.23
(1,2517)	1:190:A:GLN:H	1:190:A:GLN:HG2	18	1.23
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	6	1.23
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	20	1.23
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	12	1.23
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	17	1.23
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	13	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	15	1.23
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	2	1.23
(1,657)	1:87:A:ALA:HB1	1:88:A:LYS:HD3	11	1.23
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	10	1.23
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	18	1.23
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	15	1.23
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	15	1.23
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	13	1.23
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	16	1.23
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	11	1.22
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	1	1.22
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	16	1.22
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	10	1.22
(4,143)	1:89:A:VAL:HG22	1:10:A:LEU:HB2	17	1.22
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	4	1.22
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	9	1.22
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	3	1.22
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	4	1.22
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	14	1.22
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	20	1.22
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	7	1.22
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	19	1.22
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	10	1.22
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	9	1.22
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	5	1.22
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	10	1.22
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	3	1.22
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	19	1.22
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	5	1.22
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	12	1.22
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	8	1.22
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	19	1.22
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	7	1.22
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	5	1.22
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	12	1.21
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	19	1.21
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	7	1.21
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	4	1.21
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	3	1.21
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	14	1.21
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	15	1.21
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	16	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	5	1.21
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	18	1.21
(1,2271)	1:153:A:LYS:H	1:152:A:LYS:HB2	20	1.21
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	18	1.21
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	20	1.21
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	1	1.21
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	4	1.21
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	19	1.21
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	9	1.21
(1,1633)	1:48:A:LEU:H	1:47:A:LEU:HB2	20	1.21
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	12	1.21
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	4	1.21
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	12	1.21
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	18	1.21
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	2	1.21
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	6	1.21
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	20	1.21
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	4	1.21
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	5	1.21
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	6	1.21
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	9	1.21
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	3	1.21
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	4	1.21
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	7	1.21
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	15	1.21
(1,503)	1:57:A:ALA:HB1	1:60:A:LYS:HE2	4	1.21
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	12	1.21
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	16	1.21
(1,407)	1:36:A:LYS:HE2	1:36:A:LYS:HB3	9	1.21
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	2	1.21
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	19	1.21
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	18	1.21
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	15	1.2
(4,280)	1:179:A:ASN:H	1:178:A:VAL:HG11	14	1.2
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	11	1.2
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	5	1.2
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	6	1.2
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	13	1.2
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	15	1.2
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	14	1.2
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	3	1.2
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	13	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	5	1.2
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	15	1.2
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	16	1.2
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	6	1.2
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	1	1.2
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	3	1.2
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	7	1.2
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	2	1.2
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	14	1.2
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	14	1.2
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	19	1.2
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	5	1.2
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	5	1.2
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	7	1.2
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	3	1.2
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	1	1.2
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	7	1.2
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	18	1.2
(1,294)	1:16:A:ILE:HG12	1:121:A:LEU:HD11	18	1.2
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	8	1.2
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	2	1.19
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	17	1.19
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	14	1.19
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG21	6	1.19
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	17	1.19
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	2	1.19
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	10	1.19
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	6	1.19
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	18	1.19
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	4	1.19
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	7	1.19
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	19	1.19
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	1	1.19
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	7	1.19
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	18	1.19
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	8	1.19
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	4	1.19
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	16	1.19
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	2	1.19
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	9	1.19
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	20	1.19
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	3	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,609)	1:78:A:LEU:HD11	1:110:A:PHE:HB2	16	1.19
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	17	1.19
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	10	1.19
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	14	1.19
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	20	1.19
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	9	1.18
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	13	1.18
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	3	1.18
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	6	1.18
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	20	1.18
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD23	20	1.18
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	3	1.18
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	7	1.18
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	12	1.18
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	11	1.18
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	14	1.18
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	9	1.18
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	5	1.18
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	1	1.18
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	5	1.18
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	7	1.18
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	15	1.18
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	11	1.18
(1,1392)	1:10:A:LEU:H	1:9:A:LYS:HB3	16	1.18
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	15	1.18
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	5	1.18
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	11	1.18
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	4	1.18
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	18	1.18
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	3	1.18
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	5	1.18
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	12	1.18
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	2	1.18
(1,53)	1:185:A:ASP:HB3	1:184:A:VAL:HG22	3	1.18
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	1	1.17
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	4	1.17
(4,342)	1:29:A:GLN:H	1:187:A:VAL:HG23	8	1.17
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	15	1.17
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	20	1.17
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	19	1.17
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	1	1.17
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	5	1.17
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	2	1.17
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	10	1.17
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	1	1.17
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	6	1.17
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	9	1.17
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	10	1.17
(1,1650)	1:51:A:GLU:H	1:50:A:SER:HB2	3	1.17
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	10	1.17
(1,1182)	1:184:A:VAL:HG11	1:184:A:VAL:HA	14	1.17
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	3	1.17
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	11	1.17
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	16	1.17
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	13	1.17
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	17	1.17
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	3	1.17
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	4	1.17
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	13	1.17
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	5	1.17
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	16	1.17
(1,320)	1:19:A:VAL:HA	1:99:A:GLY:HA3	6	1.17
(1,242)	1:10:A:LEU:HB2	1:11:A:LYS:HD2	16	1.17
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	13	1.16
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	6	1.16
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	10	1.16
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	2	1.16
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	8	1.16
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	20	1.16
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	18	1.16
(1,1182)	1:184:A:VAL:HG11	1:184:A:VAL:HA	10	1.16
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	1	1.16
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	14	1.16
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	15	1.16
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	10	1.16
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	6	1.16
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	6	1.16
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	8	1.16
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	5	1.16
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	14	1.16
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	10	1.16
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	17	1.16
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	12	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	5	1.15
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	20	1.15
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	20	1.15
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	11	1.15
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	18	1.15
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	13	1.15
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	10	1.15
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	11	1.15
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	7	1.15
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	14	1.15
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	7	1.15
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	16	1.15
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	19	1.15
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	5	1.15
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	14	1.15
(1,452)	1:43:A:SER:HB2	1:45:A:GLY:HA3	3	1.15
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	4	1.15
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	12	1.15
(1,258)	1:13:A:THR:HG21	1:10:A:LEU:HD11	12	1.15
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	4	1.15
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	6	1.15
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	15	1.14
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	3	1.14
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	3	1.14
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	18	1.14
(4,138)	1:13:A:THR:HG21	1:10:A:LEU:HD23	15	1.14
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	19	1.14
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	13	1.14
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	14	1.14
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	3	1.14
(1,2499)	1:187:A:VAL:H	1:187:A:VAL:HG11	14	1.14
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	19	1.14
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	3	1.14
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	2	1.14
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	3	1.14
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	9	1.14
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	17	1.14
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	14	1.14
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	8	1.14
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	9	1.14
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	20	1.14
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	17	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	20	1.14
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	10	1.14
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	6	1.14
(1,407)	1:36:A:LYS:HE2	1:36:A:LYS:HB3	16	1.14
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	14	1.13
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	9	1.13
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	19	1.13
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	9	1.13
(4,147)	1:84:A:ALA:HB3	1:15:A:ILE:HD12	8	1.13
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	10	1.13
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	14	1.13
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	15	1.13
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	11	1.13
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	4	1.13
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	20	1.13
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	13	1.13
(1,1809)	1:77:A:VAL:H	1:73:A:PRO:HG3	11	1.13
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	5	1.13
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	6	1.13
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	12	1.13
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	18	1.13
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	4	1.12
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	7	1.12
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	4	1.12
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	18	1.12
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	1	1.12
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	8	1.12
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	3	1.12
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	13	1.12
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	16	1.12
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	5	1.12
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	4	1.12
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	20	1.12
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	13	1.12
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	4	1.12
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	20	1.12
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	6	1.12
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	2	1.12
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	12	1.12
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	13	1.12
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	19	1.12
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	20	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	11	1.12
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	14	1.12
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	9	1.12
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	7	1.12
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	10	1.12
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	12	1.12
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	13	1.12
(1,415)	1:36:A:LYS:HE3	1:188:A:PHE:HZ	13	1.12
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	8	1.12
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	9	1.12
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	7	1.12
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	3	1.12
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	16	1.12
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	16	1.11
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	7	1.11
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	19	1.11
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	10	1.11
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	14	1.11
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	7	1.11
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	3	1.11
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	18	1.11
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	12	1.11
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	1	1.11
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	3	1.11
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	19	1.11
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	2	1.11
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	5	1.11
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	18	1.11
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	5	1.11
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	19	1.11
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	20	1.11
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	10	1.11
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	1	1.11
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	5	1.11
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	7	1.11
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	19	1.11
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	8	1.11
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	2	1.11
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	5	1.11
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	9	1.11
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	14	1.11
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	7	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	13	1.1
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	6	1.1
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	8	1.1
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	7	1.1
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	11	1.1
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	11	1.1
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	19	1.1
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	5	1.1
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	11	1.1
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	14	1.1
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	16	1.1
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	2	1.1
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	11	1.1
(1,1259)	1:89:A:VAL:H	1:6:A:MET:HG2	10	1.1
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	8	1.1
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	6	1.1
(1,677)	1:89:A:VAL:HG21	1:9:A:LYS:HE2	19	1.1
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	14	1.1
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	8	1.1
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	8	1.1
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	18	1.1
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	19	1.1
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	4	1.1
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	7	1.1
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	12	1.1
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	15	1.1
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD11	12	1.09
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	14	1.09
(4,169)	1:65:A:ILE:HD13	1:68:A:LYS:HD2	18	1.09
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	8	1.09
(4,132)	1:175:A:VAL:HG23	1:166:A:ILE:H	6	1.09
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	3	1.09
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	16	1.09
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	9	1.09
(4,76)	1:10:A:LEU:HD22	1:82:A:ARG:HA	16	1.09
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	2	1.09
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	18	1.09
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	15	1.09
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	13	1.09
(1,1692)	1:59:A:GLY:H	1:54:A:SER:HB2	14	1.09
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	6	1.09
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	5	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	17	1.09
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	15	1.09
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	12	1.09
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	2	1.09
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	2	1.09
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	6	1.09
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	13	1.09
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	11	1.09
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	6	1.09
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	15	1.09
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	18	1.09
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	10	1.09
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	10	1.08
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	1	1.08
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	14	1.08
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	12	1.08
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	4	1.08
(4,107)	1:129:A:THR:HG23	1:181:A:GLU:HG2	19	1.08
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	10	1.08
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	1	1.08
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	10	1.08
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	6	1.08
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	11	1.08
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	15	1.08
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	10	1.08
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	8	1.08
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	14	1.08
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	2	1.08
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	10	1.08
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	7	1.08
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	3	1.08
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	9	1.08
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	12	1.08
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	16	1.08
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	19	1.08
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	11	1.08
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	10	1.08
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	11	1.08
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	6	1.08
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	19	1.08
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	20	1.08
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	18	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	13	1.07
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	20	1.07
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	4	1.07
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	16	1.07
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	13	1.07
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG23	1	1.07
(4,140)	1:89:A:VAL:HG22	1:86:A:VAL:HG22	12	1.07
(4,131)	1:77:A:VAL:HG23	1:100:A:TYR:HE1	7	1.07
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	5	1.07
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	15	1.07
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	12	1.07
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	6	1.07
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	14	1.07
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	16	1.07
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	3	1.07
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	14	1.07
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	12	1.07
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	12	1.07
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	1	1.07
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	5	1.07
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	13	1.07
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	18	1.07
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	3	1.07
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	13	1.07
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	11	1.07
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	8	1.07
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	18	1.07
(1,412)	1:36:A:LYS:HE3	1:37:A:TYR:HD2	16	1.07
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	11	1.07
(1,248)	1:10:A:LEU:HD21	1:7:A:GLU:HG2	12	1.07
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	8	1.07
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	16	1.07
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	7	1.06
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	11	1.06
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	15	1.06
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	9	1.06
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	3	1.06
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	5	1.06
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	6	1.06
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	14	1.06
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	19	1.06
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	17	1.06
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	4	1.06
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	17	1.06
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	4	1.06
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	19	1.06
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	9	1.06
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	9	1.06
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	6	1.06
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	4	1.06
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	5	1.06
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	12	1.06
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	3	1.06
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	16	1.06
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	7	1.06
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	15	1.06
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	1	1.06
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	20	1.06
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	3	1.06
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	4	1.06
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	17	1.06
(1,294)	1:16:A:ILE:HG12	1:121:A:LEU:HD11	6	1.06
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	16	1.06
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	8	1.06
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	6	1.06
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	10	1.05
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	15	1.05
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	2	1.05
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	10	1.05
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	8	1.05
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	13	1.05
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	8	1.05
(4,88)	1:76:A:THR:HG22	1:62:A:LEU:HB2	15	1.05
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	7	1.05
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	10	1.05
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	13	1.05
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	8	1.05
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	9	1.05
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	2	1.05
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	3	1.05
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	5	1.05
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	8	1.05
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	13	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	6	1.05
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	9	1.05
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	14	1.05
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	19	1.05
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	4	1.05
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	8	1.05
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	16	1.05
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	11	1.05
(1,806)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	12	1.05
(1,752)	1:103:A:GLU:HA	1:104:A:VAL:HG11	15	1.05
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	19	1.05
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	6	1.05
(1,238)	1:9:A:LYS:HG2	1:10:A:LEU:HD11	1	1.05
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	1	1.05
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	10	1.05
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	1	1.05
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	3	1.05
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	4	1.05
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	7	1.04
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	12	1.04
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD11	11	1.04
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	12	1.04
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD22	17	1.04
(4,199)	1:8:A:GLU:HG2	1:6:A:MET:H	13	1.04
(4,170)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	19	1.04
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	10	1.04
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	18	1.04
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	17	1.04
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	3	1.04
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	6	1.04
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	12	1.04
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	10	1.04
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	12	1.04
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	8	1.04
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	1	1.04
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	9	1.04
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	17	1.04
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	20	1.04
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	4	1.04
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	20	1.04
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	10	1.04
(1,752)	1:103:A:GLU:HA	1:104:A:VAL:HG11	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	12	1.04
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	15	1.04
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	3	1.04
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	2	1.04
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	8	1.03
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	14	1.03
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	9	1.03
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	2	1.03
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	17	1.03
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	9	1.03
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	1	1.03
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	1	1.03
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	9	1.03
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	6	1.03
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	6	1.03
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	16	1.03
(1,2202)	1:140:A:THR:H	1:141:A:SER:HB2	2	1.03
(1,2005)	1:104:A:VAL:H	1:104:A:VAL:HG11	3	1.03
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	11	1.03
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	7	1.03
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	5	1.03
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	11	1.03
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	6	1.03
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	2	1.03
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	9	1.03
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	15	1.03
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	19	1.03
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	9	1.03
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	12	1.03
(1,573)	1:73:A:PRO:HD2	1:61:A:LYS:HE3	2	1.03
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	9	1.03
(1,218)	1:156:A:GLU:HA	1:155:A:LEU:HB2	17	1.03
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	8	1.02
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD11	17	1.02
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	13	1.02
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	20	1.02
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	3	1.02
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	6	1.02
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	4	1.02
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	18	1.02
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	6	1.02
(4,132)	1:19:A:VAL:HG22	1:166:A:ILE:H	13	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,88)	1:76:A:THR:HG23	1:62:A:LEU:HB2	1	1.02
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	4	1.02
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	18	1.02
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	10	1.02
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	20	1.02
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	1	1.02
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	11	1.02
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	4	1.02
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	3	1.02
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	11	1.02
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	13	1.02
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	4	1.02
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	19	1.02
(1,902)	1:135:A:LEU:HB3	1:135:A:LEU:HD11	14	1.02
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	6	1.02
(1,865)	1:125:A:ALA:HA	1:124:A:ASP:HB2	13	1.02
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	3	1.02
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	11	1.02
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	20	1.02
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	9	1.02
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	14	1.02
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	6	1.02
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	16	1.02
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	2	1.02
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	16	1.02
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	15	1.02
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	9	1.02
(1,7)	1:10:A:LEU:HD13	1:10:A:LEU:HB2	2	1.02
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	20	1.01
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	17	1.01
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	1	1.01
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	1	1.01
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	5	1.01
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	5	1.01
(4,132)	1:175:A:VAL:HG23	1:166:A:ILE:H	12	1.01
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	19	1.01
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	17	1.01
(4,95)	1:76:A:THR:HG21	1:73:A:PRO:HG3	1	1.01
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	1	1.01
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	10	1.01
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	20	1.01
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	17	1.01
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	6	1.01
(1,2005)	1:104:A:VAL:H	1:104:A:VAL:HG11	15	1.01
(1,1436)	1:16:A:ILE:H	1:97:A:ILE:HG12	16	1.01
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	14	1.01
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	5	1.01
(1,760)	1:105:A:GLN:HA	1:104:A:VAL:HG21	15	1.01
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	12	1.01
(1,478)	1:47:A:LEU:HD11	1:84:A:ALA:HB1	12	1.01
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	3	1.01
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	10	1.01
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	11	1.01
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	18	1.01
(1,73)	1:135:A:LEU:HD12	1:139:A:GLU:HG2	9	1.01
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	17	1.0
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG22	1	1.0
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	8	1.0
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	15	1.0
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	18	1.0
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	10	1.0
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	15	1.0
(4,132)	1:19:A:VAL:HG22	1:166:A:ILE:H	20	1.0
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	9	1.0
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	18	1.0
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	16	1.0
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	15	1.0
(4,74)	1:10:A:LEU:HD21	1:95:A:PHE:HE2	2	1.0
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	2	1.0
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	15	1.0
(1,2566)	1:198:A:LEU:HD11	1:197:A:ALA:H	15	1.0
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	4	1.0
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	7	1.0
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	11	1.0
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	18	1.0
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	1	1.0
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD13	12	1.0
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	4	1.0
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	16	1.0
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	13	1.0
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	20	1.0
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	8	1.0
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	7	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	10	1.0
(1,557)	1:70:A:GLN:HG2	1:65:A:ILE:HG21	17	1.0
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	2	1.0
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	18	1.0
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	4	1.0
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	16	1.0
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	9	1.0
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	14	1.0
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	2	0.99
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	16	0.99
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD11	3	0.99
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	5	0.99
(4,211)	1:67:A:GLU:HG2	1:68:A:LYS:HE2	19	0.99
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	2	0.99
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	8	0.99
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	4	0.99
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	8	0.99
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	10	0.99
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	8	0.99
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	11	0.99
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	7	0.99
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	7	0.99
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	4	0.99
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	2	0.99
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	19	0.99
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	1	0.99
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	2	0.99
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	6	0.99
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	11	0.99
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	10	0.99
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	18	0.99
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	11	0.99
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	1	0.99
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	8	0.99
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	9	0.99
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	14	0.99
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	5	0.99
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	4	0.99
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	11	0.99
(1,566)	1:71:A:LEU:HA	1:71:A:LEU:HD21	14	0.99
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	6	0.99
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	15	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	6	0.99
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	9	0.99
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	3	0.98
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	7	0.98
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	16	0.98
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	18	0.98
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	4	0.98
(4,123)	1:125:A:ALA:HB3	1:22:A:PRO:HD2	8	0.98
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	7	0.98
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	13	0.98
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD22	16	0.98
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	16	0.98
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	5	0.98
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	11	0.98
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	18	0.98
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	2	0.98
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	4	0.98
(1,1076)	1:166:A:ILE:HD11	1:169:A:TYR:HB3	11	0.98
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	17	0.98
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	14	0.98
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	8	0.98
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	13	0.98
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	19	0.98
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	20	0.98
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	6	0.98
(1,7)	1:10:A:LEU:HD13	1:10:A:LEU:HB2	12	0.98
(4,342)	1:35:A:GLN:H	1:33:A:ILE:HG21	5	0.97
(4,298)	1:81:A:LEU:HG	1:81:A:LEU:H	2	0.97
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	9	0.97
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	3	0.97
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	13	0.97
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	1	0.97
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	13	0.97
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	8	0.97
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	14	0.97
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	16	0.97
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	19	0.97
(4,10)	1:71:A:LEU:HG	1:65:A:ILE:HG23	1	0.97
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	5	0.97
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	10	0.97
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	6	0.97
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	9	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:43:A:SER:H	1:42:A:LEU:HG	12	0.97
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	16	0.97
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	20	0.97
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	12	0.97
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	9	0.97
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	7	0.97
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	7	0.97
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	11	0.97
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	19	0.97
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	1	0.97
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	16	0.97
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	14	0.97
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	18	0.97
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	10	0.97
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	12	0.97
(1,118)	1:180:A:ALA:HB1	1:26:A:LYS:HA	6	0.97
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	8	0.97
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	14	0.97
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	20	0.97
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	7	0.96
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	11	0.96
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	17	0.96
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	17	0.96
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	16	0.96
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	5	0.96
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	19	0.96
(4,77)	1:167:A:ALA:HB2	1:170:A:GLU:HG2	2	0.96
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	6	0.96
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	8	0.96
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	13	0.96
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	12	0.96
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	20	0.96
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	5	0.96
(1,1662)	1:53:A:SER:H	1:52:A:VAL:HG21	3	0.96
(1,1622)	1:45:A:GLY:H	1:48:A:LEU:HD11	7	0.96
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	4	0.96
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	17	0.96
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	9	0.96
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	13	0.96
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	15	0.96
(1,621)	1:81:A:LEU:HB2	1:82:A:ARG:H	12	0.96
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	5	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	18	0.96
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	19	0.96
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	1	0.96
(1,382)	1:33:A:ILE:HG21	1:39:A:TYR:HB3	20	0.96
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	17	0.96
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	14	0.96
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	2	0.96
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	7	0.96
(4,355)	1:36:A:LYS:H	1:32:A:LYS:HB2	19	0.95
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	4	0.95
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	9	0.95
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	9	0.95
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	5	0.95
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	6	0.95
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	12	0.95
(4,143)	1:89:A:VAL:HG22	1:10:A:LEU:HB2	19	0.95
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	12	0.95
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	3	0.95
(4,76)	1:104:A:VAL:HG11	1:160:A:LYS:HE3	20	0.95
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	12	0.95
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	20	0.95
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	7	0.95
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	3	0.95
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	16	0.95
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	6	0.95
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	13	0.95
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	11	0.95
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	13	0.95
(1,81)	1:76:A:THR:HG21	1:58:A:ARG:HD2	17	0.95
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	10	0.94
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	1	0.94
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	5	0.94
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	6	0.94
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	11	0.94
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	13	0.94
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	8	0.94
(4,3)	1:10:A:LEU:HD13	1:13:A:THR:HA	2	0.94
(4,1)	1:78:A:LEU:HB3	1:112:A:ARG:HB2	7	0.94
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	8	0.94
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	14	0.94
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	4	0.94
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	19	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	12	0.94
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	18	0.94
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	20	0.94
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	6	0.94
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	6	0.94
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	16	0.94
(1,760)	1:105:A:GLN:HA	1:104:A:VAL:HG21	3	0.94
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	17	0.94
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	6	0.94
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	9	0.94
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	5	0.94
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	14	0.94
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	12	0.94
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	16	0.94
(1,81)	1:76:A:THR:HG22	1:58:A:ARG:HD2	18	0.94
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD12	8	0.94
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	14	0.93
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	19	0.93
(4,338)	1:52:A:VAL:HG22	1:49:A:ARG:H	6	0.93
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	5	0.93
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	6	0.93
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	20	0.93
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	13	0.93
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	2	0.93
(4,131)	1:77:A:VAL:HG22	1:100:A:TYR:HE1	16	0.93
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	20	0.93
(4,96)	1:76:A:THR:HG22	1:62:A:LEU:HD12	17	0.93
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	19	0.93
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	16	0.93
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	5	0.93
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	20	0.93
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	1	0.93
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	3	0.93
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	5	0.93
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	6	0.93
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	12	0.93
(1,1671)	1:55:A:GLY:H	1:52:A:VAL:HG21	3	0.93
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	11	0.93
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	2	0.93
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	12	0.93
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	13	0.93
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	15	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	13	0.93
(1,436)	1:41:A:HIS:HA	1:96:A:LEU:HD11	1	0.93
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	6	0.93
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	20	0.92
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	15	0.92
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	12	0.92
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	12	0.92
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	20	0.92
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	10	0.92
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	4	0.92
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	10	0.92
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	18	0.92
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	13	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	4	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	8	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	9	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	13	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	14	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	16	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	17	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	18	0.92
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	20	0.92
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	11	0.92
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	3	0.92
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	12	0.92
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	18	0.92
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	17	0.92
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	20	0.92
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	12	0.92
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	19	0.92
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	3	0.92
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	12	0.92
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	13	0.92
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	8	0.92
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	1	0.92
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	6	0.91
(4,211)	1:67:A:GLU:HG2	1:68:A:LYS:HE2	12	0.91
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	15	0.91
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	4	0.91
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	7	0.91
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	3	0.91
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	14	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	3	0.91
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	6	0.91
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	9	0.91
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	14	0.91
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	20	0.91
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	10	0.91
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	2	0.91
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	10	0.91
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	11	0.91
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	15	0.91
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	1	0.91
(1,1536)	1:34:A:VAL:H	1:35:A:GLN:HG2	12	0.91
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	10	0.91
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	19	0.91
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	18	0.91
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	9	0.91
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	11	0.91
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	3	0.91
(1,350)	1:26:A:LYS:HE3	1:22:A:PRO:HA	19	0.91
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	13	0.91
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	9	0.91
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	17	0.91
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	20	0.9
(4,339)	1:80:A:MET:H	1:84:A:ALA:HB1	20	0.9
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	3	0.9
(4,298)	1:81:A:LEU:H	1:84:A:ALA:HB1	8	0.9
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	11	0.9
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	1	0.9
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	5	0.9
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	11	0.9
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	17	0.9
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	9	0.9
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	20	0.9
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	16	0.9
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	6	0.9
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	17	0.9
(4,35)	1:61:A:LYS:HD2	1:58:A:ARG:HA	17	0.9
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	17	0.9
(1,2511)	1:189:A:SER:H	1:189:A:SER:HB3	2	0.9
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	7	0.9
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	20	0.9
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	2	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	7	0.9
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	19	0.9
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	6	0.9
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	4	0.9
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	12	0.9
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	11	0.9
(1,788)	1:114:A:ILE:HD11	1:78:A:LEU:HD11	16	0.9
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	11	0.9
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	8	0.9
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	8	0.9
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	4	0.9
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	16	0.9
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	3	0.9
(1,30)	1:6:A:MET:HA	1:6:A:MET:HG2	10	0.9
(4,126)	1:140:A:THR:HG23	1:137:A:ARG:HB2	19	0.89
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	2	0.89
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	3	0.89
(4,80)	1:78:A:LEU:HD22	1:81:A:LEU:HD23	1	0.89
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	19	0.89
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	9	0.89
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	18	0.89
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	20	0.89
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	2	0.89
(1,1536)	1:34:A:VAL:H	1:35:A:GLN:HG2	11	0.89
(1,1525)	1:32:A:LYS:H	1:32:A:LYS:HG2	6	0.89
(1,1475)	1:20:A:GLY:H	1:26:A:LYS:HE2	13	0.89
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	2	0.89
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	18	0.89
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	7	0.89
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	13	0.89
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	17	0.89
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	1	0.89
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	6	0.89
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	12	0.89
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	18	0.89
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	3	0.89
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	5	0.89
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	6	0.89
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	12	0.89
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	6	0.88
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	5	0.88
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	7	0.88
(4,146)	1:161:A:ALA:HB1	1:162:A:THR:HG1	12	0.88
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	12	0.88
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	4	0.88
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	8	0.88
(4,32)	1:113:A:ARG:HG3	1:113:A:ARG:HA	11	0.88
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	5	0.88
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	19	0.88
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	7	0.88
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	6	0.88
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	16	0.88
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	4	0.88
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	19	0.88
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	2	0.88
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	14	0.88
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	15	0.88
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	16	0.88
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	16	0.88
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	1	0.88
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	8	0.88
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	1	0.88
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	9	0.88
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	13	0.88
(1,415)	1:36:A:LYS:HE3	1:188:A:PHE:HZ	2	0.88
(1,401)	1:35:A:GLN:HA	1:36:A:LYS:HB2	9	0.88
(1,81)	1:76:A:THR:HG22	1:58:A:ARG:HD2	13	0.88
(1,30)	1:6:A:MET:HA	1:6:A:MET:HG2	12	0.88
(4,400)	1:40:A:THR:H	1:96:A:LEU:HD12	1	0.87
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	14	0.87
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	18	0.87
(4,126)	1:144:A:VAL:HG12	1:22:A:PRO:HG2	6	0.87
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	11	0.87
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	15	0.87
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	6	0.87
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	11	0.87
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	3	0.87
(4,50)	1:160:A:LYS:HG3	1:160:A:LYS:HE2	5	0.87
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	6	0.87
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	10	0.87
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	20	0.87
(4,32)	1:113:A:ARG:HG3	1:113:A:ARG:HA	4	0.87
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	11	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	12	0.87
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	11	0.87
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	19	0.87
(1,2111)	1:121:A:LEU:H	1:120:A:LEU:HD11	19	0.87
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	8	0.87
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	6	0.87
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	17	0.87
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	12	0.87
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	4	0.87
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	8	0.87
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	12	0.87
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	9	0.87
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	14	0.87
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	20	0.87
(1,730)	1:97:A:ILE:HG21	1:100:A:TYR:HB3	15	0.87
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	10	0.87
(1,401)	1:35:A:GLN:HA	1:36:A:LYS:HB2	16	0.87
(1,319)	1:19:A:VAL:HA	1:26:A:LYS:HE2	10	0.87
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	14	0.87
(1,118)	1:180:A:ALA:HB2	1:26:A:LYS:HA	5	0.87
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	10	0.87
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	13	0.87
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	4	0.87
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	2	0.86
(4,200)	1:156:A:GLU:HG3	1:153:A:LYS:HG2	3	0.86
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	6	0.86
(4,107)	1:44:A:THR:HG22	1:77:A:VAL:HB	5	0.86
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	1	0.86
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	4	0.86
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	6	0.86
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	7	0.86
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	2	0.86
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	12	0.86
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	3	0.86
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	18	0.86
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	13	0.86
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	5	0.86
(1,1883)	1:85:A:MET:H	1:86:A:VAL:HG21	12	0.86
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	8	0.86
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	12	0.86
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	15	0.86
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	18	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:34:A:VAL:H	1:35:A:GLN:HG2	3	0.86
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	20	0.86
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	5	0.86
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	18	0.86
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	9	0.86
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	20	0.86
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	18	0.86
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	18	0.86
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	10	0.86
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	20	0.86
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	12	0.86
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	17	0.86
(1,32)	1:6:A:MET:HA	1:9:A:LYS:HE2	6	0.86
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	10	0.85
(4,296)	1:46:A:ASP:H	1:48:A:LEU:HD11	20	0.85
(4,287)	1:163:A:GLU:H	1:161:A:ALA:HB2	16	0.85
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	14	0.85
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	17	0.85
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	5	0.85
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	16	0.85
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	6	0.85
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	5	0.85
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	15	0.85
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	12	0.85
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	18	0.85
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	18	0.85
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	16	0.85
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	7	0.85
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	17	0.85
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	16	0.85
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	19	0.85
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	16	0.85
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	15	0.85
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	17	0.85
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	18	0.85
(1,1002)	1:155:A:LEU:HB3	1:154:A:ARG:HB2	7	0.85
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	1	0.85
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	3	0.85
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	11	0.85
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	2	0.85
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	4	0.85
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	16	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	4	0.85
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	14	0.85
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	7	0.85
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	10	0.85
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	3	0.85
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	13	0.85
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	7	0.85
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	4	0.85
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	15	0.84
(4,315)	1:82:A:ARG:H	1:86:A:VAL:HG21	4	0.84
(4,234)	1:186:A:SER:HB2	1:185:A:ASP:HB2	2	0.84
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	10	0.84
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG21	8	0.84
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG23	9	0.84
(4,198)	1:77:A:VAL:HA	1:72:A:VAL:HB	16	0.84
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	18	0.84
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	5	0.84
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	6	0.84
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	18	0.84
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	20	0.84
(4,126)	1:144:A:VAL:HG13	1:70:A:GLN:HB2	10	0.84
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	8	0.84
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	10	0.84
(4,95)	1:76:A:THR:HG23	1:73:A:PRO:HG3	13	0.84
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	9	0.84
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	4	0.84
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	14	0.84
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	10	0.84
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	15	0.84
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	15	0.84
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	19	0.84
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	15	0.84
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	1	0.84
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	16	0.84
(1,942)	1:144:A:VAL:HG21	1:145:A:ASP:HA	16	0.84
(1,911)	1:136:A:LYS:HB2	1:136:A:LYS:HE2	11	0.84
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	17	0.84
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	1	0.84
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	11	0.84
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	14	0.84
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	18	0.84
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	5	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	7	0.84
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	6	0.84
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	15	0.84
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	14	0.84
(4,387)	1:99:A:GLY:H	1:43:A:SER:HA	11	0.83
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	7	0.83
(4,250)	1:34:A:VAL:HB	1:31:A:GLU:HA	5	0.83
(4,234)	1:189:A:SER:HA	1:192:A:CYS:HB2	4	0.83
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	7	0.83
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	2	0.83
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	4	0.83
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	7	0.83
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	15	0.83
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	3	0.83
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	15	0.83
(4,50)	1:160:A:LYS:HG3	1:160:A:LYS:HE2	13	0.83
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	13	0.83
(1,2459)	1:180:A:ALA:H	1:181:A:GLU:HB3	5	0.83
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	1	0.83
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	18	0.83
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	17	0.83
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	5	0.83
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	12	0.83
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	10	0.83
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	17	0.83
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	5	0.83
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	16	0.83
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	15	0.83
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	19	0.83
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	14	0.83
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	6	0.83
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	12	0.83
(1,782)	1:112:A:ARG:HB2	1:113:A:ARG:HD2	1	0.83
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	14	0.83
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	18	0.83
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	6	0.83
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	11	0.83
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	3	0.83
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	10	0.83
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	14	0.83
(1,256)	1:13:A:THR:HG21	1:9:A:LYS:HB3	16	0.83
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG23	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	11	0.83
(4,387)	1:99:A:GLY:H	1:43:A:SER:HA	8	0.82
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	9	0.82
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	3	0.82
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	1	0.82
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	15	0.82
(4,126)	1:144:A:VAL:HG13	1:70:A:GLN:HB2	20	0.82
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	3	0.82
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	5	0.82
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	18	0.82
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	13	0.82
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	19	0.82
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	4	0.82
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	9	0.82
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	12	0.82
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	10	0.82
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	19	0.82
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	4	0.82
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	8	0.82
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	17	0.82
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	4	0.82
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	4	0.82
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	8	0.82
(1,2190)	1:138:A:GLY:H	1:136:A:LYS:HE3	1	0.82
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	15	0.82
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	17	0.82
(1,1199)	1:188:A:PHE:HA	1:190:A:GLN:HG2	18	0.82
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	8	0.82
(1,749)	1:103:A:GLU:HG3	1:105:A:GLN:HB3	3	0.82
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	17	0.82
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	12	0.82
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	2	0.82
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	13	0.82
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	1	0.82
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	3	0.82
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	7	0.82
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	6	0.82
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	16	0.82
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	9	0.82
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	11	0.82
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	12	0.82
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	12	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,377)	1:172:A:ARG:H	1:117:A:PRO:HB3	2	0.81
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	18	0.81
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	11	0.81
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	7	0.81
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	8	0.81
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	3	0.81
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	1	0.81
(4,88)	1:76:A:THR:HG23	1:62:A:LEU:HB2	14	0.81
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	20	0.81
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	19	0.81
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	4	0.81
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	3	0.81
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	7	0.81
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	3	0.81
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	6	0.81
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	20	0.81
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	19	0.81
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	5	0.81
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	12	0.81
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	13	0.81
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	4	0.81
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	20	0.81
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	3	0.81
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	6	0.81
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	11	0.81
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	11	0.81
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	13	0.81
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	9	0.81
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	14	0.81
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	3	0.81
(1,683)	1:91:A:THR:HA	1:90:A:ASN:HB2	5	0.81
(1,663)	1:88:A:LYS:HD3	1:88:A:LYS:HA	3	0.81
(1,615)	1:79:A:ASP:HB3	1:80:A:MET:HG3	2	0.81
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	2	0.81
(1,519)	1:61:A:LYS:HD2	1:62:A:LEU:HA	17	0.81
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	4	0.81
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	7	0.81
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG22	19	0.81
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	1	0.81
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	15	0.8
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	7	0.8
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	9	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	16	0.8
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	1	0.8
(4,87)	1:195:A:LEU:HD13	1:39:A:TYR:HD2	15	0.8
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	7	0.8
(4,80)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	11	0.8
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	8	0.8
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	6	0.8
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	9	0.8
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	2	0.8
(4,35)	1:61:A:LYS:HD2	1:58:A:ARG:HA	15	0.8
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	4	0.8
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	4	0.8
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	5	0.8
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	7	0.8
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	16	0.8
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	4	0.8
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	7	0.8
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	12	0.8
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	10	0.8
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	13	0.8
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	15	0.8
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	1	0.8
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	5	0.8
(1,501)	1:57:A:ALA:HB1	1:60:A:LYS:HB2	15	0.8
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	9	0.8
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	12	0.8
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	16	0.8
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	3	0.8
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	17	0.8
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	1	0.8
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	12	0.8
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	15	0.8
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	19	0.8
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	11	0.79
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	12	0.79
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	5	0.79
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	10	0.79
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	6	0.79
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	11	0.79
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	6	0.79
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	11	0.79
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	15	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	14	0.79
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	1	0.79
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	14	0.79
(4,50)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	11	0.79
(1,2486)	1:185:A:ASP:H	1:184:A:VAL:HG21	10	0.79
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	20	0.79
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	12	0.79
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	17	0.79
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	19	0.79
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	5	0.79
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	6	0.79
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	20	0.79
(1,2191)	1:138:A:GLY:H	1:137:A:ARG:HB2	3	0.79
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	11	0.79
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	17	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	1	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	2	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	5	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	8	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	10	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	13	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	15	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	18	0.79
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	19	0.79
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	1	0.79
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	17	0.79
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	6	0.79
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	10	0.79
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	4	0.79
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	13	0.79
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	2	0.79
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	1	0.79
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	2	0.79
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	5	0.79
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	20	0.79
(1,553)	1:68:A:LYS:HD2	1:67:A:GLU:HG2	2	0.79
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	5	0.79
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	16	0.79
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	2	0.79
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	11	0.79
(1,350)	1:26:A:LYS:HE3	1:22:A:PRO:HA	2	0.79
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	5	0.79
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	11	0.79
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	12	0.79
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	20	0.79
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	2	0.79
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	7	0.79
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG22	4	0.79
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	8	0.79
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	13	0.79
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	12	0.78
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	6	0.78
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	16	0.78
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	6	0.78
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	14	0.78
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	4	0.78
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	10	0.78
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	11	0.78
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	13	0.78
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	4	0.78
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	9	0.78
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	20	0.78
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	14	0.78
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	7	0.78
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	15	0.78
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	7	0.78
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	3	0.78
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	8	0.78
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	16	0.78
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	20	0.78
(1,1379)	1:7:A:GLU:H	1:7:A:GLU:HB3	18	0.78
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	17	0.78
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	11	0.78
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	14	0.78
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	19	0.78
(1,874)	1:127:A:PRO:HG2	1:126:A:GLY:HA2	5	0.78
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	12	0.78
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	17	0.78
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	15	0.78
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	8	0.78
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	16	0.78
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	9	0.78
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	20	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	6	0.78
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	9	0.78
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	10	0.78
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	11	0.78
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	18	0.78
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	11	0.78
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	15	0.78
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	18	0.78
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	7	0.78
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	18	0.77
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	3	0.77
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	8	0.77
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	18	0.77
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	19	0.77
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	4	0.77
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	9	0.77
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	11	0.77
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	1	0.77
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	15	0.77
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	13	0.77
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	17	0.77
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	17	0.77
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	13	0.77
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	11	0.77
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	19	0.77
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	15	0.77
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	19	0.77
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	9	0.77
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	2	0.77
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	16	0.77
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	12	0.77
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	18	0.77
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	10	0.77
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	18	0.77
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	10	0.77
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	12	0.77
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	8	0.77
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	4	0.77
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	17	0.77
(1,1729)	1:64:A:GLU:H	1:65:A:ILE:HG13	10	0.77
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	9	0.77
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	17	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	15	0.77
(1,1210)	1:192:A:CYS:HB2	1:196:A:ASP:HB3	2	0.77
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	17	0.77
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	4	0.77
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	5	0.77
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	18	0.77
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	1	0.77
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	10	0.77
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	14	0.77
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	11	0.77
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	20	0.77
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	19	0.77
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	4	0.77
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	14	0.77
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	19	0.77
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	5	0.77
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	6	0.77
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	6	0.77
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	17	0.77
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG13	19	0.77
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	18	0.77
(1,59)	1:62:A:LEU:HD13	1:58:A:ARG:HD2	4	0.77
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	14	0.76
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	13	0.76
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	5	0.76
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	13	0.76
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	1	0.76
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	19	0.76
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	9	0.76
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	16	0.76
(4,144)	1:89:A:VAL:HG23	1:6:A:MET:H	2	0.76
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	7	0.76
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	19	0.76
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	15	0.76
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	15	0.76
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	20	0.76
(4,35)	1:61:A:LYS:HD2	1:58:A:ARG:HA	7	0.76
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	5	0.76
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	12	0.76
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	11	0.76
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	4	0.76
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	14	0.76
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	9	0.76
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	9	0.76
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	2	0.76
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	6	0.76
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	3	0.76
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	12	0.76
(1,1202)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	18	0.76
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	8	0.76
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	2	0.76
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	2	0.76
(1,862)	1:124:A:ASP:HB2	1:122:A:TYR:HB2	14	0.76
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	19	0.76
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	4	0.76
(1,680)	1:89:A:VAL:HG21	1:90:A:ASN:HD21	20	0.76
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	9	0.76
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	7	0.76
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	15	0.76
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	2	0.76
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	18	0.76
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	1	0.76
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	14	0.76
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	10	0.75
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	4	0.75
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	7	0.75
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	7	0.75
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	8	0.75
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	17	0.75
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	18	0.75
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	4	0.75
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	5	0.75
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	13	0.75
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	1	0.75
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	8	0.75
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	9	0.75
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	9	0.75
(4,74)	1:10:A:LEU:HD22	1:95:A:PHE:HE2	12	0.75
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	2	0.75
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	16	0.75
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	19	0.75
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	5	0.75
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	12	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	15	0.75
(1,2572)	1:198:A:LEU:H	1:198:A:LEU:HD11	15	0.75
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	14	0.75
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	1	0.75
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	11	0.75
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	16	0.75
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	11	0.75
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	14	0.75
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	15	0.75
(1,2084)	1:116:A:GLN:H	1:111:A:GLU:HG2	11	0.75
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	11	0.75
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	7	0.75
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	10	0.75
(1,1519)	1:31:A:GLU:H	1:31:A:GLU:HB3	14	0.75
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	14	0.75
(1,1379)	1:7:A:GLU:H	1:7:A:GLU:HB3	11	0.75
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	4	0.75
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	15	0.75
(1,1169)	1:180:A:ALA:HA	1:187:A:VAL:HG11	14	0.75
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	6	0.75
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	7	0.75
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	10	0.75
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	12	0.75
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	13	0.75
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	14	0.75
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	3	0.75
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	10	0.75
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	5	0.75
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	13	0.75
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	6	0.75
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	17	0.75
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	9	0.75
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	11	0.75
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	14	0.75
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	17	0.75
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	17	0.75
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	13	0.75
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	16	0.75
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	15	0.75
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	10	0.75
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	13	0.75
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	14	0.75
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	3	0.74
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	16	0.74
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	14	0.74
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	16	0.74
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	17	0.74
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	11	0.74
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	15	0.74
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	3	0.74
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	4	0.74
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	10	0.74
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	14	0.74
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	8	0.74
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	6	0.74
(1,2486)	1:185:A:ASP:H	1:184:A:VAL:HG21	14	0.74
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	11	0.74
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	17	0.74
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	13	0.74
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	13	0.74
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	19	0.74
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	14	0.74
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	5	0.74
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	10	0.74
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	5	0.74
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	10	0.74
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	12	0.74
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	5	0.74
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	10	0.74
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	2	0.74
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	4	0.74
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	10	0.74
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	8	0.74
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	3	0.74
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	2	0.74
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG21	14	0.74
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	16	0.74
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	8	0.74
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	20	0.73
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	1	0.73
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	7	0.73
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	19	0.73
(4,273)	1:167:A:ALA:HB1	1:164:A:PRO:HD2	16	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	2	0.73
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	19	0.73
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	15	0.73
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	7	0.73
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	15	0.73
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	3	0.73
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	9	0.73
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	16	0.73
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	2	0.73
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	9	0.73
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	20	0.73
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	9	0.73
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	8	0.73
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	1	0.73
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	2	0.73
(1,1379)	1:7:A:GLU:H	1:7:A:GLU:HB3	2	0.73
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	6	0.73
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	9	0.73
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	1	0.73
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	3	0.73
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	14	0.73
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	20	0.73
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	3	0.73
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	15	0.73
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	17	0.73
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	18	0.73
(1,902)	1:135:A:LEU:HB3	1:135:A:LEU:HD11	9	0.73
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	7	0.73
(1,780)	1:112:A:ARG:HA	1:112:A:ARG:HD2	1	0.73
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	6	0.73
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	12	0.73
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	19	0.73
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	4	0.73
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	17	0.73
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	13	0.73
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	15	0.73
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	5	0.73
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	7	0.73
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	5	0.73
(1,206)	1:72:A:VAL:HA	1:72:A:VAL:HG22	16	0.73
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	6	0.73
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	14	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,399)	1:98:A:ASP:H	1:96:A:LEU:HA	1	0.72
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	16	0.72
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	18	0.72
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	3	0.72
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	9	0.72
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	13	0.72
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	2	0.72
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	9	0.72
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	5	0.72
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	6	0.72
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	1	0.72
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	11	0.72
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	5	0.72
(4,273)	1:167:A:ALA:HB1	1:164:A:PRO:HD2	9	0.72
(4,273)	1:167:A:ALA:HB1	1:164:A:PRO:HD2	10	0.72
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	16	0.72
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	17	0.72
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	20	0.72
(4,198)	1:52:A:VAL:HA	1:58:A:ARG:HG2	7	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	2	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	3	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	9	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	13	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	17	0.72
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	18	0.72
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	13	0.72
(4,149)	1:161:A:ALA:HB1	1:165:A:VAL:HG22	3	0.72
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	11	0.72
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	5	0.72
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	19	0.72
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	20	0.72
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	10	0.72
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	6	0.72
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	17	0.72
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	11	0.72
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	5	0.72
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	11	0.72
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	15	0.72
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	9	0.72
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	5	0.72
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	17	0.72
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	13	0.72
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	4	0.72
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	1	0.72
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	18	0.72
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	20	0.72
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	2	0.72
(1,582)	1:74:A:LEU:HD11	1:74:A:LEU:HA	17	0.72
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	16	0.72
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	16	0.72
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	19	0.72
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	18	0.72
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	3	0.72
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	4	0.72
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	15	0.72
(1,301)	1:16:A:ILE:HG21	1:119:A:LEU:HB2	15	0.72
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	17	0.72
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	4	0.72
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	6	0.72
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	12	0.72
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	6	0.71
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	17	0.71
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	5	0.71
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	6	0.71
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	8	0.71
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	17	0.71
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	17	0.71
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	17	0.71
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	6	0.71
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	7	0.71
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	14	0.71
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	19	0.71
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	20	0.71
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	8	0.71
(4,200)	1:148:A:GLU:HG3	1:131:A:THR:HG23	19	0.71
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	4	0.71
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	6	0.71
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	14	0.71
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	16	0.71
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	20	0.71
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	4	0.71
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	19	0.71
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	13	0.71
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	1	0.71
(4,126)	1:144:A:VAL:HG11	1:154:A:ARG:HB3	14	0.71
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	5	0.71
(4,95)	1:76:A:THR:HG21	1:73:A:PRO:HG3	7	0.71
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	18	0.71
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	4	0.71
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	8	0.71
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	9	0.71
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	18	0.71
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	16	0.71
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	1	0.71
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	4	0.71
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	8	0.71
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	8	0.71
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	20	0.71
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	3	0.71
(1,2206)	1:141:A:SER:H	1:141:A:SER:HB2	2	0.71
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	5	0.71
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	4	0.71
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	5	0.71
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	16	0.71
(1,2074)	1:113:A:ARG:H	1:114:A:ILE:HG12	7	0.71
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	15	0.71
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	17	0.71
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	15	0.71
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	4	0.71
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	10	0.71
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	11	0.71
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	18	0.71
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	17	0.71
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	19	0.71
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	16	0.71
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	7	0.71
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	8	0.71
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	20	0.71
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	1	0.71
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	17	0.71
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	17	0.71
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	10	0.71
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	6	0.71
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	6	0.71
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	8	0.71
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	17	0.71
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	18	0.71
(1,415)	1:36:A:LYS:HE3	1:188:A:PHE:HZ	9	0.71
(1,412)	1:36:A:LYS:HE3	1:37:A:TYR:HD2	9	0.71
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	20	0.71
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	8	0.71
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	18	0.71
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	11	0.71
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	3	0.7
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	9	0.7
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	12	0.7
(4,369)	1:183:A:SER:H	1:187:A:VAL:HG11	8	0.7
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	10	0.7
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	16	0.7
(4,340)	1:80:A:MET:H	1:76:A:THR:HG21	2	0.7
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	14	0.7
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	15	0.7
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	16	0.7
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	9	0.7
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG22	10	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	1	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	2	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	4	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	11	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	13	0.7
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	18	0.7
(4,219)	1:65:A:ILE:HA	1:72:A:VAL:HG22	10	0.7
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	10	0.7
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	7	0.7
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	3	0.7
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	4	0.7
(4,92)	1:76:A:THR:HG21	1:80:A:MET:HG3	17	0.7
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	7	0.7
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	9	0.7
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	16	0.7
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	9	0.7
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	7	0.7
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	4	0.7
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	7	0.7
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	6	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	5	0.7
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	10	0.7
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	8	0.7
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	12	0.7
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	1	0.7
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	8	0.7
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	7	0.7
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	20	0.7
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	1	0.7
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	15	0.7
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	2	0.7
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	7	0.7
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	8	0.7
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	13	0.7
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	18	0.7
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	2	0.7
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	2	0.7
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	11	0.7
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	11	0.7
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	16	0.7
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	20	0.7
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	12	0.7
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	1	0.7
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	2	0.7
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	17	0.7
(1,680)	1:89:A:VAL:HG21	1:90:A:ASN:HD21	16	0.7
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	17	0.7
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	13	0.7
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	5	0.7
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	15	0.7
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	7	0.7
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	19	0.7
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	2	0.7
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	10	0.7
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	5	0.7
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	15	0.7
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	20	0.7
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	1	0.7
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	10	0.7
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	17	0.7
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	20	0.7
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	5	0.69
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	20	0.69
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	2	0.69
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	10	0.69
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	20	0.69
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	15	0.69
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	17	0.69
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	3	0.69
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	5	0.69
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	12	0.69
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	5	0.69
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	5	0.69
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	8	0.69
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	10	0.69
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	12	0.69
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	9	0.69
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	17	0.69
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	9	0.69
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	12	0.69
(4,107)	1:129:A:THR:HG23	1:181:A:GLU:HG2	4	0.69
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	1	0.69
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	13	0.69
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	19	0.69
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	12	0.69
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	9	0.69
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	10	0.69
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	10	0.69
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	12	0.69
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	2	0.69
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	3	0.69
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	6	0.69
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	10	0.69
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	7	0.69
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	12	0.69
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	16	0.69
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	2	0.69
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	16	0.69
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	20	0.69
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	11	0.69
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	1	0.69
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	15	0.69
(1,1265)	1:145:A:ASP:H	1:143:A:ARG:HB2	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	1	0.69
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	18	0.69
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	1	0.69
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	3	0.69
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	1	0.69
(1,888)	1:131:A:THR:HG21	1:132:A:GLN:HG2	4	0.69
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	18	0.69
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	4	0.69
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	14	0.69
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	17	0.69
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	3	0.69
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	6	0.69
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	4	0.69
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	9	0.69
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	13	0.69
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	14	0.69
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	1	0.69
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	1	0.69
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	3	0.69
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	3	0.69
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	8	0.69
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	11	0.69
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	13	0.69
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	9	0.69
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	20	0.68
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	17	0.68
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	12	0.68
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	2	0.68
(4,222)	1:48:A:LEU:HA	1:51:A:GLU:HG2	14	0.68
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	16	0.68
(4,192)	1:118:A:THR:HB	1:174:A:ILE:HG23	1	0.68
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	14	0.68
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	9	0.68
(4,133)	1:19:A:VAL:HG22	1:169:A:TYR:HD1	3	0.68
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	6	0.68
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	12	0.68
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	17	0.68
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	13	0.68
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	13	0.68
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	20	0.68
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	4	0.68
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	5	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	11	0.68
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	14	0.68
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	16	0.68
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	20	0.68
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	4	0.68
(1,2419)	1:177:A:LYS:H	1:176:A:ARG:HD2	3	0.68
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	4	0.68
(1,2383)	1:171:A:LYS:H	1:172:A:ARG:HD3	10	0.68
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	18	0.68
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	7	0.68
(1,2121)	1:122:A:TYR:H	1:177:A:LYS:HG3	8	0.68
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	2	0.68
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	7	0.68
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	9	0.68
(1,2080)	1:114:A:ILE:H	1:114:A:ILE:HG12	14	0.68
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	2	0.68
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	9	0.68
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	16	0.68
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	10	0.68
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	9	0.68
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	20	0.68
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	6	0.68
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	9	0.68
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	3	0.68
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	9	0.68
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	9	0.68
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	19	0.68
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	3	0.68
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	10	0.68
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	12	0.68
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	4	0.68
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	16	0.68
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	3	0.68
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	8	0.68
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	5	0.68
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	3	0.68
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	2	0.68
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	4	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	1	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	2	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	3	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	5	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	6	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	7	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	8	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	9	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	10	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	11	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	12	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	13	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	14	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	15	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	16	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	17	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	18	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	19	0.68
(1,516)	1:60:A:LYS:HA	1:60:A:LYS:HB3	20	0.68
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	12	0.68
(1,464)	1:44:A:THR:HG21	1:81:A:LEU:HB3	19	0.68
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	2	0.68
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	19	0.68
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	3	0.68
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	9	0.68
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	7	0.68
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	9	0.68
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	15	0.68
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	19	0.68
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	7	0.67
(4,377)	1:172:A:ARG:H	1:117:A:PRO:HB3	16	0.67
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG23	19	0.67
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	5	0.67
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	3	0.67
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	8	0.67
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	12	0.67
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	15	0.67
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	6	0.67
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	3	0.67
(4,185)	1:198:A:LEU:HB3	1:198:A:LEU:HD22	9	0.67
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	11	0.67
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	16	0.67
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	3	0.67
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	8	0.67
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	11	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	14	0.67
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	18	0.67
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	20	0.67
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	14	0.67
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	14	0.67
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	1	0.67
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	7	0.67
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	12	0.67
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	2	0.67
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	20	0.67
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	19	0.67
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	8	0.67
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	16	0.67
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	9	0.67
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	20	0.67
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	4	0.67
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	10	0.67
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	13	0.67
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	7	0.67
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	10	0.67
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	4	0.67
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	14	0.67
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	17	0.67
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	19	0.67
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	1	0.67
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	14	0.67
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	16	0.67
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	19	0.67
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	11	0.67
(1,958)	1:149:A:GLU:HG3	1:149:A:GLU:HA	20	0.67
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	18	0.67
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	13	0.67
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	9	0.67
(1,551)	1:68:A:LYS:HA	1:70:A:GLN:HG2	20	0.67
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	10	0.67
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	3	0.67
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	1	0.67
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	13	0.67
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	3	0.67
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	11	0.67
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	15	0.67
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	17	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	7	0.67
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	12	0.67
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	3	0.67
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	19	0.67
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	1	0.67
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	4	0.66
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	6	0.66
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	8	0.66
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	13	0.66
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	14	0.66
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	3	0.66
(4,353)	1:85:A:MET:H	1:6:A:MET:HG2	6	0.66
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	4	0.66
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD13	10	0.66
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB1	13	0.66
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	14	0.66
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	18	0.66
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	12	0.66
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	12	0.66
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	14	0.66
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	6	0.66
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	1	0.66
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	18	0.66
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	11	0.66
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	15	0.66
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	2	0.66
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	15	0.66
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	16	0.66
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	18	0.66
(4,62)	1:78:A:LEU:HD23	1:78:A:LEU:HA	16	0.66
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	13	0.66
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	7	0.66
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	2	0.66
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	3	0.66
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	8	0.66
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	11	0.66
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	19	0.66
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	5	0.66
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	13	0.66
(1,2179)	1:135:A:LEU:H	1:135:A:LEU:HB2	14	0.66
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	7	0.66
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	14	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	5	0.66
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	15	0.66
(1,1350)	1:55:A:GLY:H	1:62:A:LEU:HD11	5	0.66
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	20	0.66
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	20	0.66
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	14	0.66
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	14	0.66
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	14	0.66
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	5	0.66
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	18	0.66
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	16	0.66
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	10	0.66
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	5	0.66
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	1	0.66
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	15	0.66
(1,735)	1:99:A:GLY:HA3	1:26:A:LYS:HG3	16	0.66
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	6	0.66
(1,582)	1:74:A:LEU:HD11	1:74:A:LEU:HA	11	0.66
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	18	0.66
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	14	0.66
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	19	0.66
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	20	0.66
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	4	0.65
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	14	0.65
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	19	0.65
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	20	0.65
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	11	0.65
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	19	0.65
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	18	0.65
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	9	0.65
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	20	0.65
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	3	0.65
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	4	0.65
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	13	0.65
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	4	0.65
(4,273)	1:167:A:ALA:HB1	1:166:A:ILE:HA	8	0.65
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	4	0.65
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	14	0.65
(4,219)	1:65:A:ILE:HA	1:72:A:VAL:HG22	3	0.65
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	14	0.65
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	14	0.65
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	20	0.65
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	5	0.65
(4,50)	1:160:A:LYS:HG3	1:160:A:LYS:HE2	14	0.65
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	6	0.65
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	19	0.65
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	10	0.65
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG22	20	0.65
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	13	0.65
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	17	0.65
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	18	0.65
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	5	0.65
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	9	0.65
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	14	0.65
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	11	0.65
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	15	0.65
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	19	0.65
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	1	0.65
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	7	0.65
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	4	0.65
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	12	0.65
(1,1927)	1:92:A:SER:H	1:88:A:LYS:HB3	20	0.65
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	1	0.65
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	12	0.65
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	12	0.65
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	3	0.65
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	7	0.65
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	7	0.65
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD12	6	0.65
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	4	0.65
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	5	0.65
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	6	0.65
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	15	0.65
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	20	0.65
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	10	0.65
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	6	0.65
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	15	0.65
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	13	0.65
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	1	0.65
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	7	0.65
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	8	0.65
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	4	0.65
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:6:A:MET:HA	1:9:A:LYS:HE2	7	0.65
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	4	0.65
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	15	0.64
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	17	0.64
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	7	0.64
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	18	0.64
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	4	0.64
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	18	0.64
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	3	0.64
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	8	0.64
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG22	8	0.64
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	8	0.64
(4,219)	1:65:A:ILE:HA	1:72:A:VAL:HG21	7	0.64
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	9	0.64
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	13	0.64
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	7	0.64
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	20	0.64
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	7	0.64
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	14	0.64
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	8	0.64
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	6	0.64
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	18	0.64
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	2	0.64
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	12	0.64
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	18	0.64
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	19	0.64
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	15	0.64
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	10	0.64
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	8	0.64
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	18	0.64
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	2	0.64
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	8	0.64
(1,1263)	1:145:A:ASP:H	1:151:A:ILE:HD13	8	0.64
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	4	0.64
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	17	0.64
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	20	0.64
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	20	0.64
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	6	0.64
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	19	0.64
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	8	0.64
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	12	0.64
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	14	0.64
(1,508)	1:58:A:ARG:HD2	1:51:A:GLU:HB3	15	0.64
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	19	0.64
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	20	0.64
(1,249)	1:10:A:LEU:HD21	1:11:A:LYS:HD3	2	0.64
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	4	0.64
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	1	0.64
(1,40)	1:114:A:ILE:HG13	1:97:A:ILE:HD13	2	0.64
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	3	0.64
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	12	0.64
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	1	0.63
(4,340)	1:80:A:MET:H	1:76:A:THR:HG21	5	0.63
(4,338)	1:48:A:LEU:HD21	1:49:A:ARG:H	9	0.63
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	10	0.63
(4,269)	1:132:A:GLN:HA	1:132:A:GLN:HB2	11	0.63
(4,269)	1:132:A:GLN:HA	1:132:A:GLN:HB2	18	0.63
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	3	0.63
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	4	0.63
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	9	0.63
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	4	0.63
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	19	0.63
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	11	0.63
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	15	0.63
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	14	0.63
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	9	0.63
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	2	0.63
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	19	0.63
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	7	0.63
(1,2471)	1:182:A:GLY:H	1:181:A:GLU:HG2	4	0.63
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	8	0.63
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	3	0.63
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	14	0.63
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	20	0.63
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	17	0.63
(1,2016)	1:105:A:GLN:H	1:105:A:GLN:HG3	15	0.63
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	13	0.63
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	5	0.63
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	1	0.63
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG21	16	0.63
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	17	0.63
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	6	0.63
(1,592)	1:77:A:VAL:HA	1:48:A:LEU:HD21	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	20	0.63
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	17	0.63
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	4	0.63
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	9	0.63
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	10	0.63
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	8	0.63
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	20	0.63
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	19	0.62
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	3	0.62
(4,377)	1:172:A:ARG:H	1:117:A:PRO:HB3	15	0.62
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	5	0.62
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	13	0.62
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	11	0.62
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	15	0.62
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	16	0.62
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	9	0.62
(4,217)	1:47:A:LEU:HD13	1:43:A:SER:HB3	8	0.62
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	11	0.62
(4,88)	1:76:A:THR:HG23	1:73:A:PRO:HB3	20	0.62
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	6	0.62
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	11	0.62
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	19	0.62
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	8	0.62
(4,50)	1:160:A:LYS:HG3	1:160:A:LYS:HE2	19	0.62
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	15	0.62
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	3	0.62
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	9	0.62
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	4	0.62
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	12	0.62
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	14	0.62
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	8	0.62
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	2	0.62
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	4	0.62
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	5	0.62
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	9	0.62
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	6	0.62
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	8	0.62
(1,1408)	1:13:A:THR:H	1:12:A:LYS:HG2	4	0.62
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	1	0.62
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG21	10	0.62
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	2	0.62
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	9	0.62
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	15	0.62
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	14	0.62
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	9	0.62
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	13	0.62
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	13	0.62
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	13	0.62
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	17	0.62
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	5	0.62
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	2	0.62
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	13	0.62
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	4	0.62
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	14	0.62
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	16	0.62
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	19	0.62
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	20	0.62
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	5	0.62
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	15	0.62
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	9	0.62
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	10	0.62
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	11	0.62
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	15	0.62
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	2	0.61
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	5	0.61
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	11	0.61
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	17	0.61
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	2	0.61
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	10	0.61
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	2	0.61
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	2	0.61
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	16	0.61
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	2	0.61
(4,237)	1:171:A:LYS:HB2	1:168:A:PHE:HA	15	0.61
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	4	0.61
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	18	0.61
(4,185)	1:135:A:LEU:HB3	1:135:A:LEU:HD12	14	0.61
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	19	0.61
(4,143)	1:89:A:VAL:HG23	1:10:A:LEU:HB2	10	0.61
(4,107)	1:28:A:THR:HG21	1:32:A:LYS:HB2	13	0.61
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	9	0.61
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	10	0.61
(4,50)	1:88:A:LYS:HG3	1:88:A:LYS:HE2	16	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	1	0.61
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	2	0.61
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	12	0.61
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	10	0.61
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	1	0.61
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	7	0.61
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	9	0.61
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	12	0.61
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	7	0.61
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	14	0.61
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	6	0.61
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	10	0.61
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	1	0.61
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	18	0.61
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	11	0.61
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	8	0.61
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	10	0.61
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	16	0.61
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	19	0.61
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	14	0.61
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	20	0.61
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG21	2	0.61
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	17	0.61
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	18	0.61
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	6	0.61
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	13	0.61
(1,832)	1:121:A:LEU:HB3	1:16:A:ILE:HD11	5	0.61
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	9	0.61
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	7	0.61
(1,612)	1:78:A:LEU:HD21	1:106:A:GLN:HG3	11	0.61
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	5	0.61
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	16	0.61
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	8	0.61
(1,115)	1:104:A:VAL:HG23	1:105:A:GLN:HB2	3	0.61
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	14	0.61
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	3	0.61
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	17	0.61
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	2	0.61
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	6	0.61
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	14	0.61
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	15	0.61
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	11	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	10	0.6
(4,377)	1:172:A:ARG:H	1:117:A:PRO:HB3	13	0.6
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	14	0.6
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	20	0.6
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	19	0.6
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	16	0.6
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	5	0.6
(4,308)	1:64:A:GLU:H	1:62:A:LEU:HB3	6	0.6
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	14	0.6
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	12	0.6
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	6	0.6
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	12	0.6
(4,211)	1:67:A:GLU:HG2	1:68:A:LYS:HE2	17	0.6
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	10	0.6
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	4	0.6
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	8	0.6
(4,146)	1:161:A:ALA:HB2	1:162:A:THR:HG1	17	0.6
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	10	0.6
(4,44)	1:160:A:LYS:HA	1:164:A:PRO:HD2	4	0.6
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	10	0.6
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	6	0.6
(1,2571)	1:198:A:LEU:H	1:198:A:LEU:HB2	15	0.6
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	17	0.6
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	6	0.6
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	12	0.6
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	14	0.6
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	9	0.6
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	11	0.6
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	17	0.6
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	4	0.6
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	9	0.6
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	19	0.6
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	12	0.6
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	12	0.6
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	14	0.6
(1,888)	1:131:A:THR:HG21	1:132:A:GLN:HG2	6	0.6
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	13	0.6
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	1	0.6
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	18	0.6
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	18	0.6
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	2	0.6
(1,518)	1:60:A:LYS:HD3	1:61:A:LYS:HB3	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	16	0.6
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	2	0.6
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	19	0.6
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	2	0.6
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	4	0.6
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	7	0.6
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	15	0.6
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	20	0.6
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	13	0.6
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	19	0.6
(4,399)	1:98:A:ASP:H	1:41:A:HIS:HA	2	0.59
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	18	0.59
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	6	0.59
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	3	0.59
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	5	0.59
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	13	0.59
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD12	19	0.59
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD1	13	0.59
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	16	0.59
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	13	0.59
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	13	0.59
(4,44)	1:160:A:LYS:HA	1:164:A:PRO:HD2	19	0.59
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	7	0.59
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	19	0.59
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	16	0.59
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	5	0.59
(1,2481)	1:184:A:VAL:H	1:184:A:VAL:HG11	10	0.59
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	14	0.59
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	2	0.59
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	18	0.59
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	16	0.59
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	18	0.59
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	17	0.59
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	16	0.59
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	5	0.59
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	7	0.59
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	14	0.59
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	5	0.59
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	16	0.59
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	12	0.59
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	6	0.59
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	5	0.59
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	7	0.59
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	2	0.59
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	10	0.59
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	16	0.59
(1,782)	1:112:A:ARG:HB2	1:113:A:ARG:HD2	6	0.59
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	4	0.59
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	9	0.59
(1,461)	1:44:A:THR:HG21	1:47:A:LEU:HB2	20	0.59
(1,341)	1:134:A:LEU:HD11	1:23:A:GLY:HA2	4	0.59
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	5	0.59
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	18	0.59
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	11	0.59
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	17	0.59
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	4	0.59
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	17	0.58
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	10	0.58
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	1	0.58
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	8	0.58
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	6	0.58
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	2	0.58
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	11	0.58
(4,126)	1:144:A:VAL:HG13	1:154:A:ARG:HB3	16	0.58
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	19	0.58
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	15	0.58
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	3	0.58
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	16	0.58
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	1	0.58
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	19	0.58
(1,2481)	1:184:A:VAL:H	1:184:A:VAL:HG11	14	0.58
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	7	0.58
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	19	0.58
(1,2218)	1:143:A:ARG:H	1:146:A:ASP:HB2	15	0.58
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	4	0.58
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	13	0.58
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	1	0.58
(1,1678)	1:56:A:SER:H	1:56:A:SER:HB2	13	0.58
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	11	0.58
(1,1365)	1:59:A:GLY:H	1:57:A:ALA:HB2	13	0.58
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG21	8	0.58
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	19	0.58
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	20	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	5	0.58
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	1	0.58
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	4	0.58
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	7	0.58
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	12	0.58
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	18	0.58
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	10	0.58
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	13	0.58
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	1	0.58
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	2	0.58
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	2	0.58
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	11	0.58
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	1	0.58
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	4	0.58
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	1	0.58
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG23	12	0.58
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	11	0.58
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	18	0.58
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	13	0.58
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	7	0.58
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	13	0.58
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	18	0.58
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	16	0.57
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD13	18	0.57
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	14	0.57
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	11	0.57
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	10	0.57
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	12	0.57
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	2	0.57
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	17	0.57
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	12	0.57
(4,143)	1:89:A:VAL:HG22	1:10:A:LEU:HB2	12	0.57
(4,133)	1:175:A:VAL:HG21	1:169:A:TYR:HD1	17	0.57
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	20	0.57
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	13	0.57
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	5	0.57
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	18	0.57
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	4	0.57
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	5	0.57
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	14	0.57
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	9	0.57
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	20	0.57
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	10	0.57
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	15	0.57
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	17	0.57
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	20	0.57
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	20	0.57
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	3	0.57
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	2	0.57
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	13	0.57
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	5	0.57
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	3	0.57
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	2	0.57
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	13	0.57
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	16	0.57
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	13	0.57
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	7	0.57
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	3	0.57
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	9	0.57
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	3	0.57
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	9	0.57
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	13	0.57
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	6	0.57
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	8	0.57
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	7	0.57
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	9	0.57
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	18	0.57
(1,43)	1:190:A:GLN:HA	1:190:A:GLN:HG2	18	0.57
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	5	0.57
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	16	0.57
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	17	0.57
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	7	0.57
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	10	0.56
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	7	0.56
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	18	0.56
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	2	0.56
(4,338)	1:49:A:ARG:H	1:48:A:LEU:HD12	7	0.56
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	12	0.56
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	8	0.56
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	2	0.56
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD1	2	0.56
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	5	0.56
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	14	0.56
(4,211)	1:67:A:GLU:HG2	1:68:A:LYS:HE2	11	0.56
(4,196)	1:131:A:THR:HA	1:151:A:ILE:HG22	4	0.56
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	7	0.56
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	13	0.56
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	10	0.56
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	6	0.56
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	14	0.56
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	16	0.56
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	18	0.56
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	10	0.56
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	4	0.56
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	11	0.56
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	14	0.56
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	10	0.56
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	6	0.56
(1,2423)	1:177:A:LYS:H	1:177:A:LYS:HD3	5	0.56
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	4	0.56
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	11	0.56
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	4	0.56
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	13	0.56
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	3	0.56
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	3	0.56
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	8	0.56
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG23	3	0.56
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	20	0.56
(1,1285)	1:8:A:GLU:H	1:8:A:GLU:HG2	2	0.56
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	20	0.56
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	20	0.56
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	7	0.56
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	12	0.56
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	16	0.56
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	7	0.56
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	2	0.56
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	2	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	1	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	2	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	3	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	4	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	5	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	6	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	8	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	9	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	10	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	11	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	12	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG21	13	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	14	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	15	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	16	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	17	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG23	18	0.56
(1,126)	1:15:A:ILE:HG21	1:15:A:ILE:HG23	19	0.56
(1,126)	1:15:A:ILE:HG22	1:15:A:ILE:HG21	20	0.56
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	17	0.56
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	8	0.56
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	12	0.55
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	6	0.55
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	9	0.55
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	11	0.55
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	7	0.55
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	12	0.55
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	4	0.55
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	8	0.55
(4,313)	1:190:A:GLN:H	1:186:A:SER:HA	14	0.55
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	15	0.55
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	19	0.55
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	19	0.55
(4,126)	1:144:A:VAL:HG11	1:154:A:ARG:HB3	2	0.55
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	17	0.55
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	20	0.55
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	20	0.55
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	2	0.55
(4,32)	1:113:A:ARG:HG3	1:79:A:ASP:HA	2	0.55
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	11	0.55
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	16	0.55
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	7	0.55
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	8	0.55
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	9	0.55
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	15	0.55
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	5	0.55
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	3	0.55
(1,2279)	1:154:A:ARG:H	1:154:A:ARG:HB3	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	5	0.55
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	1	0.55
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	3	0.55
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	4	0.55
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	4	0.55
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	1	0.55
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	5	0.55
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	20	0.55
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	4	0.55
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG23	8	0.55
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	15	0.55
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	6	0.55
(1,1315)	1:85:A:MET:H	1:88:A:LYS:HZ2	16	0.55
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	8	0.55
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	13	0.55
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	18	0.55
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	13	0.55
(1,749)	1:103:A:GLU:HG3	1:105:A:GLN:HB3	1	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	6	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	10	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	12	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	14	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	15	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	17	0.55
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	18	0.55
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	10	0.55
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	19	0.55
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	18	0.55
(1,14)	1:195:A:LEU:HD21	1:37:A:TYR:HE2	12	0.55
(4,387)	1:99:A:GLY:H	1:18:A:VAL:HA	1	0.54
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	7	0.54
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	16	0.54
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	14	0.54
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	11	0.54
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	17	0.54
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	3	0.54
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	11	0.54
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	12	0.54
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	9	0.54
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	11	0.54
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	20	0.54
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	9	0.54
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	7	0.54
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	13	0.54
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	12	0.54
(4,71)	1:118:A:THR:HG22	1:94:A:GLY:HA2	20	0.54
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	11	0.54
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	1	0.54
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	9	0.54
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	5	0.54
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	5	0.54
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	6	0.54
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	8	0.54
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	14	0.54
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	8	0.54
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	4	0.54
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	10	0.54
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	17	0.54
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	5	0.54
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	11	0.54
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	20	0.54
(1,2013)	1:105:A:GLN:H	1:104:A:VAL:HG21	3	0.54
(1,2013)	1:105:A:GLN:H	1:104:A:VAL:HG21	15	0.54
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	12	0.54
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	6	0.54
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	7	0.54
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	13	0.54
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	12	0.54
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	5	0.54
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	6	0.54
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	9	0.54
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	14	0.54
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	11	0.54
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	6	0.54
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	12	0.54
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	16	0.54
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	4	0.54
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	20	0.54
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	4	0.54
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	8	0.54
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	8	0.54
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	9	0.54
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	20	0.54
(1,484)	1:49:A:ARG:HD2	1:49:A:ARG:HA	12	0.54
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	15	0.54
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	16	0.54
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	1	0.54
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	11	0.54
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	8	0.54
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	12	0.54
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	15	0.54
(1,73)	1:135:A:LEU:HD13	1:139:A:GLU:HG2	15	0.54
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	5	0.54
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG12	17	0.54
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	3	0.54
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	14	0.53
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	17	0.53
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	8	0.53
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	5	0.53
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	12	0.53
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	19	0.53
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	18	0.53
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	11	0.53
(4,321)	1:86:A:VAL:H	1:82:A:ARG:HB3	20	0.53
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	1	0.53
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	5	0.53
(4,296)	1:46:A:ASP:H	1:47:A:LEU:HD13	8	0.53
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	11	0.53
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	1	0.53
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	16	0.53
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	17	0.53
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	20	0.53
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	1	0.53
(4,96)	1:76:A:THR:HG23	1:62:A:LEU:HD12	12	0.53
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	2	0.53
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	16	0.53
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	17	0.53
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	18	0.53
(4,66)	1:86:A:VAL:HG12	1:6:A:MET:H	5	0.53
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	4	0.53
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	12	0.53
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	13	0.53
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	18	0.53
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	13	0.53
(1,2476)	1:183:A:SER:H	1:182:A:GLY:HA2	13	0.53
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	2	0.53
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	13	0.53
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	13	0.53
(1,2159)	1:128:A:GLU:H	1:128:A:GLU:HG3	1	0.53
(1,2089)	1:116:A:GLN:H	1:116:A:GLN:HG2	16	0.53
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	13	0.53
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG23	9	0.53
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	11	0.53
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	14	0.53
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	18	0.53
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	3	0.53
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	7	0.53
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	3	0.53
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	2	0.53
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	20	0.53
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	16	0.53
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	1	0.53
(1,488)	1:50:A:SER:HB2	1:80:A:MET:HE1	18	0.53
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	1	0.53
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	4	0.53
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	9	0.53
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	20	0.53
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	5	0.53
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	7	0.53
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	16	0.53
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	9	0.53
(1,386)	1:34:A:VAL:HA	1:39:A:TYR:HB3	15	0.53
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	9	0.53
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	16	0.53
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	13	0.53
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	8	0.53
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	15	0.53
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	1	0.53
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	5	0.53
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	6	0.53
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	12	0.53
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	5	0.52
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	20	0.52
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	6	0.52
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	7	0.52
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	2	0.52
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	8	0.52
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	17	0.52
(4,308)	1:61:A:LYS:H	1:62:A:LEU:HD22	7	0.52
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	6	0.52
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	17	0.52
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	4	0.52
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	15	0.52
(4,256)	1:137:A:ARG:HB3	1:134:A:LEU:HA	15	0.52
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	13	0.52
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	9	0.52
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	9	0.52
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	20	0.52
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	5	0.52
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	9	0.52
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	2	0.52
(4,144)	1:89:A:VAL:HG23	1:9:A:LYS:HG2	4	0.52
(4,81)	1:10:A:LEU:HD23	1:118:A:THR:HB	13	0.52
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	5	0.52
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	9	0.52
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	15	0.52
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	19	0.52
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	15	0.52
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	5	0.52
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	11	0.52
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	17	0.52
(1,2218)	1:143:A:ARG:H	1:146:A:ASP:HB2	2	0.52
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	12	0.52
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	6	0.52
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	19	0.52
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	12	0.52
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	11	0.52
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	15	0.52
(1,1328)	1:50:A:SER:H	1:51:A:GLU:HG2	12	0.52
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	13	0.52
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	6	0.52
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	7	0.52
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	3	0.52
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	15	0.52
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	6	0.52
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	2	0.52
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	9	0.52
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	3	0.52
(1,778)	1:111:A:GLU:HG3	1:117:A:PRO:HG2	2	0.52
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	10	0.52
(1,749)	1:103:A:GLU:HG3	1:105:A:GLN:HB3	9	0.52
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	4	0.52
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	7	0.52
(1,485)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	8	0.52
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	4	0.52
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	10	0.52
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	4	0.52
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	5	0.52
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	14	0.52
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	11	0.52
(1,115)	1:104:A:VAL:HG23	1:105:A:GLN:HB2	15	0.52
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	10	0.52
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	11	0.52
(1,66)	1:10:A:LEU:HD22	1:89:A:VAL:HG11	10	0.52
(1,62)	1:118:A:THR:HG22	1:14:A:LYS:HB3	5	0.52
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	1	0.52
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	19	0.52
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	13	0.51
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	5	0.51
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	4	0.51
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	15	0.51
(4,325)	1:160:A:LYS:H	1:160:A:LYS:HB2	1	0.51
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	18	0.51
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	19	0.51
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	9	0.51
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	20	0.51
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	10	0.51
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	19	0.51
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	2	0.51
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	7	0.51
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	14	0.51
(4,144)	1:89:A:VAL:HG23	1:9:A:LYS:HG2	15	0.51
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	12	0.51
(4,133)	1:175:A:VAL:HG23	1:169:A:TYR:HD1	8	0.51
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	19	0.51
(4,92)	1:76:A:THR:HG21	1:80:A:MET:HG3	2	0.51
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG3	13	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	3	0.51
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	20	0.51
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	7	0.51
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	16	0.51
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	12	0.51
(1,2181)	1:136:A:LYS:H	1:135:A:LEU:HB3	14	0.51
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	12	0.51
(1,1721)	1:63:A:SER:H	1:62:A:LEU:HD11	4	0.51
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	10	0.51
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	6	0.51
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	13	0.51
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	1	0.51
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	7	0.51
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	15	0.51
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	19	0.51
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	1	0.51
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	5	0.51
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	14	0.51
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	1	0.51
(1,749)	1:103:A:GLU:HG3	1:105:A:GLN:HB3	20	0.51
(1,653)	1:87:A:ALA:HB1	1:83:A:ASP:HB2	10	0.51
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	6	0.51
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	3	0.51
(1,415)	1:36:A:LYS:HE3	1:188:A:PHE:HZ	16	0.51
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	2	0.51
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	14	0.51
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	18	0.51
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	19	0.51
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	7	0.51
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	5	0.51
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	5	0.51
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	6	0.51
(1,96)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	8	0.51
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	8	0.51
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	14	0.51
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	3	0.5
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	8	0.5
(4,367)	1:119:A:LEU:H	1:117:A:PRO:HB2	1	0.5
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	4	0.5
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	4	0.5
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	15	0.5
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	6	0.5
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	10	0.5
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	10	0.5
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	3	0.5
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	20	0.5
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	9	0.5
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	3	0.5
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	12	0.5
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	16	0.5
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	17	0.5
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	19	0.5
(4,131)	1:19:A:VAL:HG22	1:100:A:TYR:HD2	18	0.5
(4,92)	1:76:A:THR:HG21	1:79:A:ASP:HB2	5	0.5
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	7	0.5
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	7	0.5
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	14	0.5
(4,35)	1:61:A:LYS:HD2	1:58:A:ARG:HA	19	0.5
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	4	0.5
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	14	0.5
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	19	0.5
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	2	0.5
(4,1)	1:74:A:LEU:HB3	1:106:A:GLN:HB2	19	0.5
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	1	0.5
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	13	0.5
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	1	0.5
(1,1774)	1:71:A:LEU:HD21	1:71:A:LEU:H	6	0.5
(1,1774)	1:71:A:LEU:HD21	1:71:A:LEU:H	16	0.5
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	15	0.5
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	3	0.5
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	18	0.5
(1,1416)	1:14:A:LYS:H	1:14:A:LYS:HG2	18	0.5
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	12	0.5
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	20	0.5
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	20	0.5
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	17	0.5
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	8	0.5
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	7	0.5
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	16	0.5
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	17	0.5
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	18	0.5
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	14	0.5
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	11	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	9	0.5
(1,510)	1:58:A:ARG:HD2	1:58:A:ARG:HB2	15	0.5
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	6	0.5
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	8	0.5
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	19	0.5
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	5	0.5
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	4	0.5
(1,129)	1:175:A:VAL:HG11	1:174:A:ILE:HD13	8	0.5
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	3	0.5
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	7	0.5
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	15	0.5
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	11	0.5
(4,401)	1:24:A:SER:H	1:130:A:MET:HE1	2	0.49
(4,401)	1:24:A:SER:H	1:134:A:LEU:HB2	20	0.49
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	8	0.49
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	11	0.49
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	19	0.49
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	3	0.49
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	9	0.49
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	8	0.49
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	19	0.49
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	2	0.49
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	15	0.49
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	4	0.49
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	7	0.49
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	13	0.49
(4,200)	1:149:A:GLU:HG3	1:153:A:LYS:HG2	6	0.49
(4,196)	1:131:A:THR:HA	1:151:A:ILE:HG22	8	0.49
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	6	0.49
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	20	0.49
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	18	0.49
(4,108)	1:178:A:VAL:HG11	1:190:A:GLN:HG3	20	0.49
(4,80)	1:78:A:LEU:HD23	1:81:A:LEU:HD23	6	0.49
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	17	0.49
(4,70)	1:118:A:THR:HG23	1:174:A:ILE:HG23	1	0.49
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	18	0.49
(4,24)	1:47:A:LEU:HG	1:44:A:THR:HA	5	0.49
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	8	0.49
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	19	0.49
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	20	0.49
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	17	0.49
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:71:A:LEU:HD21	1:71:A:LEU:H	19	0.49
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	18	0.49
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	7	0.49
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	5	0.49
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	7	0.49
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	10	0.49
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	13	0.49
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	17	0.49
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	10	0.49
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	6	0.49
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	1	0.49
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	13	0.49
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	20	0.49
(1,1001)	1:154:A:ARG:HB3	1:154:A:ARG:HD2	3	0.49
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	5	0.49
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	16	0.49
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	3	0.49
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	3	0.49
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	4	0.49
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	1	0.49
(1,227)	1:7:A:GLU:HA	1:6:A:MET:HG2	10	0.49
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	7	0.49
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	18	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	4	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	7	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	9	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	10	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	14	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	17	0.49
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	19	0.49
(4,401)	1:24:A:SER:H	1:130:A:MET:HE2	7	0.48
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	15	0.48
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	1	0.48
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	19	0.48
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	8	0.48
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	19	0.48
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	11	0.48
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	10	0.48
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	14	0.48
(4,294)	1:186:A:SER:H	1:185:A:ASP:HB3	17	0.48
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	15	0.48
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	1	0.48
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	18	0.48
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	19	0.48
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	7	0.48
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	10	0.48
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	19	0.48
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	20	0.48
(4,208)	1:156:A:GLU:HG3	1:157:A:THR:HG1	3	0.48
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	8	0.48
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	15	0.48
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	1	0.48
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	15	0.48
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	11	0.48
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	4	0.48
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	20	0.48
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	9	0.48
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	20	0.48
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	12	0.48
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	17	0.48
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	15	0.48
(1,2573)	1:198:A:LEU:H	1:199:A:LYS:HE2	4	0.48
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	4	0.48
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	13	0.48
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	4	0.48
(1,2419)	1:177:A:LYS:H	1:176:A:ARG:HD2	14	0.48
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	3	0.48
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	18	0.48
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	1	0.48
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	10	0.48
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	7	0.48
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	15	0.48
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	5	0.48
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	7	0.48
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	3	0.48
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	4	0.48
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	14	0.48
(1,1236)	1:198:A:LEU:HD11	1:199:A:LYS:HE2	10	0.48
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	16	0.48
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	10	0.48
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	6	0.48
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	1	0.48
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	19	0.48
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	4	0.48
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	5	0.48
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	7	0.48
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	16	0.48
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	20	0.48
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	16	0.48
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	9	0.48
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	20	0.48
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	16	0.48
(4,401)	1:24:A:SER:H	1:130:A:MET:HE1	10	0.47
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	4	0.47
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	10	0.47
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	16	0.47
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	16	0.47
(4,322)	1:86:A:VAL:H	1:82:A:ARG:HG2	9	0.47
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	17	0.47
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	1	0.47
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	5	0.47
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	5	0.47
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	1	0.47
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	19	0.47
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	10	0.47
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	13	0.47
(4,196)	1:131:A:THR:HA	1:151:A:ILE:HG22	3	0.47
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	12	0.47
(4,152)	1:167:A:ALA:HB1	1:166:A:ILE:HB	18	0.47
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	1	0.47
(4,73)	1:78:A:LEU:HD11	1:110:A:PHE:HE1	3	0.47
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG3	1	0.47
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	2	0.47
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	16	0.47
(4,14)	1:195:A:LEU:HD23	1:198:A:LEU:H	6	0.47
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	3	0.47
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	16	0.47
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	12	0.47
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	18	0.47
(1,2434)	1:178:A:VAL:H	1:177:A:LYS:HG3	9	0.47
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	3	0.47
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	6	0.47
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	10	0.47
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	19	0.47
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	20	0.47
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	10	0.47
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	17	0.47
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	18	0.47
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	13	0.47
(1,1641)	1:49:A:ARG:H	1:49:A:ARG:HD2	17	0.47
(1,1387)	1:9:A:LYS:H	1:8:A:GLU:HG2	2	0.47
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	18	0.47
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	1	0.47
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	16	0.47
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	4	0.47
(1,1106)	1:170:A:GLU:HB2	1:175:A:VAL:HG11	10	0.47
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	12	0.47
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	8	0.47
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	11	0.47
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	15	0.47
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	16	0.47
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	16	0.47
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	12	0.47
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	15	0.47
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	8	0.47
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	8	0.47
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	14	0.47
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	12	0.47
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	20	0.47
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	20	0.47
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	1	0.47
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	3	0.47
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	18	0.47
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	16	0.47
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	12	0.46
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	18	0.46
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	12	0.46
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	8	0.46
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	1	0.46
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	3	0.46
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	5	0.46
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	4	0.46
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	9	0.46
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	11	0.46
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	18	0.46
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	3	0.46
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	5	0.46
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	1	0.46
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	17	0.46
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	19	0.46
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	4	0.46
(4,219)	1:65:A:ILE:HA	1:71:A:LEU:HD21	11	0.46
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	12	0.46
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	3	0.46
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	18	0.46
(4,66)	1:86:A:VAL:HG12	1:6:A:MET:H	1	0.46
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	4	0.46
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	9	0.46
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	5	0.46
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	1	0.46
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	4	0.46
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	8	0.46
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	17	0.46
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	11	0.46
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	5	0.46
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	14	0.46
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	6	0.46
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	4	0.46
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	8	0.46
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	1	0.46
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	4	0.46
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	17	0.46
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	18	0.46
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	19	0.46
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	1	0.46
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	18	0.46
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	19	0.46
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	11	0.46
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	4	0.46
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	18	0.46
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	17	0.46
(1,738)	1:101:A:PRO:HA	1:102:A:ARG:HG2	20	0.46
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	18	0.46
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	11	0.46
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	4	0.46
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:43:A:SER:HB2	1:98:A:ASP:HB2	14	0.46
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	4	0.46
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	13	0.46
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	16	0.46
(1,294)	1:16:A:ILE:HG12	1:121:A:LEU:HD11	20	0.46
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	2	0.46
(1,153)	1:166:A:ILE:HD12	1:162:A:THR:HG1	18	0.46
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	16	0.46
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	20	0.46
(4,377)	1:106:A:GLN:H	1:101:A:PRO:HG2	5	0.45
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	2	0.45
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	16	0.45
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	13	0.45
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	2	0.45
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	9	0.45
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	9	0.45
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	16	0.45
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	1	0.45
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	6	0.45
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	17	0.45
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	11	0.45
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	18	0.45
(4,222)	1:67:A:GLU:HG2	1:64:A:GLU:HA	16	0.45
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	10	0.45
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	1	0.45
(4,161)	1:97:A:ILE:HG22	1:47:A:LEU:HB2	15	0.45
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	11	0.45
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	12	0.45
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	18	0.45
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	18	0.45
(1,2465)	1:181:A:GLU:H	1:181:A:GLU:HG2	19	0.45
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	8	0.45
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	9	0.45
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	15	0.45
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	16	0.45
(1,1867)	1:84:A:ALA:H	1:83:A:ASP:HB2	6	0.45
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	3	0.45
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	20	0.45
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	6	0.45
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	8	0.45
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	15	0.45
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	20	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	8	0.45
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	15	0.45
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	9	0.45
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	2	0.45
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	4	0.45
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	12	0.45
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	14	0.45
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	3	0.45
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	3	0.45
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	14	0.45
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	20	0.45
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	9	0.45
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	18	0.45
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	2	0.45
(1,249)	1:10:A:LEU:HD21	1:11:A:LYS:HD3	12	0.45
(1,248)	1:10:A:LEU:HD21	1:7:A:GLU:HG2	2	0.45
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	16	0.45
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	15	0.44
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	5	0.44
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	2	0.44
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	7	0.44
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	3	0.44
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	16	0.44
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	15	0.44
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG11	3	0.44
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	4	0.44
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	7	0.44
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	16	0.44
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HB3	1	0.44
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	2	0.44
(4,285)	1:93:A:LYS:H	1:93:A:LYS:HB3	9	0.44
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	15	0.44
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	20	0.44
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	14	0.44
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	18	0.44
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	1	0.44
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	8	0.44
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	7	0.44
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	14	0.44
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	17	0.44
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	20	0.44
(4,81)	1:10:A:LEU:HD22	1:85:A:MET:HA	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	12	0.44
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	18	0.44
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	1	0.44
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	20	0.44
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	12	0.44
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	10	0.44
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	4	0.44
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	10	0.44
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	1	0.44
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	15	0.44
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	7	0.44
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	13	0.44
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	1	0.44
(1,2292)	1:156:A:GLU:H	1:156:A:GLU:HG3	13	0.44
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	14	0.44
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	16	0.44
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	12	0.44
(1,2212)	1:142:A:GLY:H	1:143:A:ARG:HB3	17	0.44
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	2	0.44
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	7	0.44
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	12	0.44
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	16	0.44
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	5	0.44
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	9	0.44
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	10	0.44
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	10	0.44
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	4	0.44
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	10	0.44
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	18	0.44
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	17	0.44
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	6	0.44
(1,868)	1:125:A:ALA:HB1	1:24:A:SER:HB3	2	0.44
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	13	0.44
(1,594)	1:77:A:VAL:HA	1:77:A:VAL:HG11	5	0.44
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	5	0.44
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	6	0.44
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	6	0.44
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD22	11	0.44
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	20	0.44
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	11	0.44
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	16	0.44
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	12	0.43
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	19	0.43
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	7	0.43
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	14	0.43
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	7	0.43
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	5	0.43
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	19	0.43
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	20	0.43
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	16	0.43
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	6	0.43
(4,301)	1:145:A:ASP:H	1:154:A:ARG:HD3	7	0.43
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	4	0.43
(4,298)	1:81:A:LEU:H	1:84:A:ALA:HB1	20	0.43
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	16	0.43
(4,217)	1:47:A:LEU:HD11	1:43:A:SER:HB3	6	0.43
(4,217)	1:47:A:LEU:HD11	1:43:A:SER:HB3	17	0.43
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	6	0.43
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	18	0.43
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	20	0.43
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	7	0.43
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG3	17	0.43
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	13	0.43
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	1	0.43
(4,21)	1:22:A:PRO:HG3	1:143:A:ARG:HD2	7	0.43
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	15	0.43
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	10	0.43
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	2	0.43
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	5	0.43
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	11	0.43
(1,2363)	1:168:A:PHE:H	1:168:A:PHE:HB3	14	0.43
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	2	0.43
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	3	0.43
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	16	0.43
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	14	0.43
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	4	0.43
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	5	0.43
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	8	0.43
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	17	0.43
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	20	0.43
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	17	0.43
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	8	0.43
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	12	0.43
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG23	16	0.43
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	4	0.43
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	14	0.43
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	17	0.43
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	7	0.43
(1,1254)	1:100:A:TYR:H	1:26:A:LYS:HD3	12	0.43
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	9	0.43
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	20	0.43
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	19	0.43
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	7	0.43
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	9	0.43
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	16	0.43
(1,917)	1:137:A:ARG:HD3	1:137:A:ARG:HB2	19	0.43
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	5	0.43
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	19	0.43
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	15	0.43
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	3	0.43
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	12	0.43
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	20	0.43
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	1	0.43
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD22	17	0.43
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	6	0.43
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	9	0.43
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	10	0.43
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	18	0.42
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	11	0.42
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	12	0.42
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	6	0.42
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG22	1	0.42
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	17	0.42
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	6	0.42
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	10	0.42
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	11	0.42
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	20	0.42
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	10	0.42
(4,286)	1:151:A:ILE:H	1:153:A:LYS:HE2	4	0.42
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	1	0.42
(4,276)	1:170:A:GLU:H	1:169:A:TYR:HD2	8	0.42
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	8	0.42
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	20	0.42
(4,151)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,151)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	15	0.42
(4,151)	1:49:A:ARG:HG2	1:49:A:ARG:HD2	18	0.42
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	3	0.42
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	8	0.42
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	9	0.42
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	14	0.42
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	17	0.42
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	2	0.42
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	16	0.42
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	1	0.42
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	5	0.42
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	3	0.42
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	8	0.42
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	18	0.42
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	3	0.42
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	4	0.42
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	8	0.42
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	17	0.42
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	8	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	3	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	6	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	10	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	11	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	13	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	14	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	15	0.42
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	18	0.42
(1,1867)	1:84:A:ALA:H	1:83:A:ASP:HB2	5	0.42
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	17	0.42
(1,1704)	1:60:A:LYS:H	1:61:A:LYS:HG2	4	0.42
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	2	0.42
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	4	0.42
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	9	0.42
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	14	0.42
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	19	0.42
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	11	0.42
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	6	0.42
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	18	0.42
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	5	0.42
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	16	0.42
(1,1286)	1:148:A:GLU:H	1:151:A:ILE:HG13	4	0.42
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	7	0.42
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	1	0.42
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	8	0.42
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	13	0.42
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	19	0.42
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	5	0.42
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	10	0.42
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	14	0.42
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	15	0.42
(1,782)	1:112:A:ARG:HB2	1:113:A:ARG:HD2	16	0.42
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	3	0.42
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	2	0.42
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	6	0.42
(1,583)	1:75:A:GLU:HG2	1:74:A:LEU:HD11	11	0.42
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	2	0.42
(1,491)	1:52:A:VAL:HA	1:52:A:VAL:HG11	3	0.42
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	16	0.42
(1,341)	1:134:A:LEU:HD11	1:23:A:GLY:HA2	8	0.42
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	16	0.42
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	6	0.42
(1,227)	1:7:A:GLU:HA	1:6:A:MET:HG2	12	0.42
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	3	0.42
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	6	0.42
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	3	0.42
(1,1)	1:14:A:LYS:HG3	1:14:A:LYS:HA	13	0.42
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	15	0.41
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	11	0.41
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	5	0.41
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	10	0.41
(4,379)	1:37:A:TYR:H	1:36:A:LYS:HG2	6	0.41
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	4	0.41
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	5	0.41
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	9	0.41
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	16	0.41
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	20	0.41
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	11	0.41
(4,347)	1:40:A:THR:H	1:96:A:LEU:HB2	13	0.41
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	14	0.41
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	20	0.41
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	2	0.41
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	10	0.41
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	7	0.41
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	16	0.41
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	3	0.41
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	6	0.41
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	9	0.41
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	1	0.41
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	20	0.41
(4,57)	1:19:A:VAL:HG12	1:19:A:VAL:HB	18	0.41
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	2	0.41
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	5	0.41
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	11	0.41
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	8	0.41
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	15	0.41
(1,2293)	1:156:A:GLU:H	1:159:A:TYR:HB3	19	0.41
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	18	0.41
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	1	0.41
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	13	0.41
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	15	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	1	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	2	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	4	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	7	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	9	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	16	0.41
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	19	0.41
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	5	0.41
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	10	0.41
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	16	0.41
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	3	0.41
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	9	0.41
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	11	0.41
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	3	0.41
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	13	0.41
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	8	0.41
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	19	0.41
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	15	0.41
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	7	0.41
(1,999)	1:154:A:ARG:HB3	1:151:A:ILE:HA	7	0.41
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	3	0.41
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	20	0.41
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	15	0.41
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	19	0.41
(1,695)	1:94:A:GLY:HA3	1:199:A:LYS:HE3	15	0.41
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	7	0.41
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	12	0.41
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	1	0.41
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	15	0.41
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	19	0.41
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	20	0.41
(1,294)	1:16:A:ILE:HG12	1:121:A:LEU:HD11	11	0.41
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	11	0.41
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	3	0.41
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	9	0.41
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	11	0.41
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	10	0.41
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	14	0.41
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	2	0.41
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	1	0.4
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	4	0.4
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	15	0.4
(4,394)	1:8:A:GLU:H	1:8:A:GLU:HA	20	0.4
(4,383)	1:23:A:GLY:H	1:134:A:LEU:HB3	12	0.4
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	4	0.4
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	20	0.4
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	11	0.4
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	19	0.4
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	17	0.4
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	15	0.4
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	7	0.4
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	12	0.4
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	4	0.4
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	10	0.4
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	6	0.4
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	9	0.4
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	15	0.4
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	17	0.4
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	13	0.4
(4,248)	1:123:A:VAL:HA	1:124:A:ASP:HB3	5	0.4
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	3	0.4
(4,199)	1:149:A:GLU:HG3	1:152:A:LYS:HB3	15	0.4
(4,152)	1:167:A:ALA:HB3	1:170:A:GLU:HB2	10	0.4
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	13	0.4
(4,95)	1:76:A:THR:HG23	1:73:A:PRO:HG3	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,81)	1:10:A:LEU:HD22	1:85:A:MET:HA	1	0.4
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	12	0.4
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	17	0.4
(4,34)	1:114:A:ILE:HG12	1:85:A:MET:HG2	10	0.4
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	3	0.4
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	5	0.4
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	18	0.4
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	10	0.4
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	13	0.4
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	12	0.4
(1,2549)	1:196:A:ASP:H	1:194:A:HIS:HB2	8	0.4
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	16	0.4
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	20	0.4
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	10	0.4
(1,2249)	1:148:A:GLU:H	1:148:A:GLU:HB2	20	0.4
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	14	0.4
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	20	0.4
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	17	0.4
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	20	0.4
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	3	0.4
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	16	0.4
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	5	0.4
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	20	0.4
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	5	0.4
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	7	0.4
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	8	0.4
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	9	0.4
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	12	0.4
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	17	0.4
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	15	0.4
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	9	0.4
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	3	0.4
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	10	0.4
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	8	0.4
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	13	0.4
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	5	0.4
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	12	0.4
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	1	0.4
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	13	0.4
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	18	0.4
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	11	0.4
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	7	0.4
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	2	0.4
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	7	0.4
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	9	0.4
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	2	0.39
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	6	0.39
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	9	0.39
(4,352)	1:141:A:SER:H	1:137:A:ARG:HB3	8	0.39
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	5	0.39
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	10	0.39
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	19	0.39
(4,322)	1:86:A:VAL:H	1:82:A:ARG:HG2	15	0.39
(4,313)	1:190:A:GLN:H	1:178:A:VAL:HA	7	0.39
(4,296)	1:46:A:ASP:H	1:47:A:LEU:HD11	6	0.39
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	10	0.39
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	12	0.39
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	18	0.39
(4,112)	1:134:A:LEU:HD11	1:137:A:ARG:HD2	15	0.39
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	1	0.39
(4,66)	1:106:A:GLN:HB3	1:78:A:LEU:HD21	10	0.39
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	10	0.39
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	13	0.39
(4,44)	1:190:A:GLN:HA	1:189:A:SER:HB3	16	0.39
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	7	0.39
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	8	0.39
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	16	0.39
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	1	0.39
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	3	0.39
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	16	0.39
(1,2439)	1:179:A:ASN:H	1:177:A:LYS:HB2	14	0.39
(1,2427)	1:178:A:VAL:H	1:122:A:TYR:HB2	9	0.39
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	5	0.39
(1,1955)	1:95:A:PHE:H	1:95:A:PHE:HB3	12	0.39
(1,1867)	1:84:A:ALA:H	1:83:A:ASP:HB2	20	0.39
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	10	0.39
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	6	0.39
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	11	0.39
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	19	0.39
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	12	0.39
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	12	0.39
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	2	0.39
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	1	0.39
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	11	0.39
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	17	0.39
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	4	0.39
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	9	0.39
(1,937)	1:144:A:VAL:HB	1:145:A:ASP:HB2	16	0.39
(1,839)	1:121:A:LEU:HD11	1:176:A:ARG:HB2	8	0.39
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	8	0.39
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	3	0.39
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	11	0.39
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	20	0.39
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	1	0.39
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	1	0.39
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	11	0.39
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	18	0.39
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	13	0.39
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	15	0.39
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	10	0.39
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	18	0.39
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	7	0.39
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE1	17	0.39
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	2	0.39
(1,81)	1:76:A:THR:HG23	1:58:A:ARG:HD2	1	0.39
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	18	0.39
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	14	0.38
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	2	0.38
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	10	0.38
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	15	0.38
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	12	0.38
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	14	0.38
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	15	0.38
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	16	0.38
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	17	0.38
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	5	0.38
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	17	0.38
(4,266)	1:108:A:GLU:HA	1:108:A:GLU:HB2	19	0.38
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	4	0.38
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	8	0.38
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	12	0.38
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	2	0.38
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	7	0.38
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	6	0.38
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	7	0.38
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	8	0.38
(4,88)	1:76:A:THR:HG23	1:62:A:LEU:HB2	10	0.38
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	5	0.38
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	1	0.38
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	13	0.38
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	19	0.38
(4,57)	1:19:A:VAL:HG12	1:19:A:VAL:HB	20	0.38
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	9	0.38
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	6	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	1	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	3	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	4	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	5	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	12	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	14	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	18	0.38
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	20	0.38
(4,10)	1:29:A:GLN:HB2	1:187:A:VAL:HG23	8	0.38
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	18	0.38
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	11	0.38
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	15	0.38
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	13	0.38
(1,1498)	1:27:A:GLY:H	1:26:A:LYS:HD3	16	0.38
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	19	0.38
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	6	0.38
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	9	0.38
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	14	0.38
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	3	0.38
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	16	0.38
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	12	0.38
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	4	0.38
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	6	0.38
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	8	0.38
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	19	0.38
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	20	0.38
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	18	0.38
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	11	0.38
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	18	0.38
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	1	0.38
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	4	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	4	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	6	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	14	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	15	0.38
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	16	0.38
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	10	0.38
(1,547)	1:67:A:GLU:HG2	1:66:A:MET:HG2	5	0.38
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	19	0.38
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	18	0.38
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	7	0.38
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	5	0.38
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	7	0.38
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	14	0.38
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	15	0.38
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	17	0.38
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	19	0.38
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	12	0.38
(1,47)	1:198:A:LEU:HA	1:199:A:LYS:HE2	5	0.38
(1,32)	1:6:A:MET:HA	1:9:A:LYS:HE2	19	0.38
(4,401)	1:24:A:SER:H	1:130:A:MET:HE1	9	0.37
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	3	0.37
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	9	0.37
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	3	0.37
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	4	0.37
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	12	0.37
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	2	0.37
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	14	0.37
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	13	0.37
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	14	0.37
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	7	0.37
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	12	0.37
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	11	0.37
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	4	0.37
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	6	0.37
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	9	0.37
(4,144)	1:89:A:VAL:HG23	1:6:A:MET:H	10	0.37
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	16	0.37
(4,92)	1:76:A:THR:HG21	1:80:A:MET:HG3	19	0.37
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	16	0.37
(4,81)	1:10:A:LEU:HD21	1:85:A:MET:HA	2	0.37
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	9	0.37
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	16	0.37
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	7	0.37
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	15	0.37
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	11	0.37
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	13	0.37
(1,2490)	1:185:A:ASP:H	1:186:A:SER:HB2	20	0.37
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	20	0.37
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	9	0.37
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	8	0.37
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	19	0.37
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	17	0.37
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	7	0.37
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	13	0.37
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	4	0.37
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	18	0.37
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	6	0.37
(1,1303)	1:147:A:ASN:H	1:150:A:THR:HG22	7	0.37
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	14	0.37
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	12	0.37
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	9	0.37
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	13	0.37
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	1	0.37
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	4	0.37
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	5	0.37
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	5	0.37
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	12	0.37
(1,818)	1:119:A:LEU:HA	1:120:A:LEU:HG	19	0.37
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	4	0.37
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	2	0.37
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	5	0.37
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	13	0.37
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	19	0.37
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	4	0.37
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	5	0.37
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	16	0.37
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	11	0.37
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	6	0.37
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	20	0.37
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	20	0.37
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	9	0.37
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	13	0.37
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	14	0.37
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	10	0.37
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	4	0.37
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	20	0.37
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	1	0.36
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	2	0.36
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	12	0.36
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	5	0.36
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	15	0.36
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	13	0.36
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	9	0.36
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	17	0.36
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	2	0.36
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	8	0.36
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	1	0.36
(4,318)	1:65:A:ILE:H	1:62:A:LEU:HA	4	0.36
(4,313)	1:190:A:GLN:H	1:186:A:SER:HA	18	0.36
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	7	0.36
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	19	0.36
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	15	0.36
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	6	0.36
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	2	0.36
(4,222)	1:67:A:GLU:HG2	1:64:A:GLU:HA	11	0.36
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	4	0.36
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	6	0.36
(4,57)	1:19:A:VAL:HG12	1:19:A:VAL:HB	7	0.36
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	10	0.36
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	12	0.36
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	15	0.36
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	2	0.36
(4,16)	1:195:A:LEU:HD23	1:195:A:LEU:HB2	9	0.36
(1,2448)	1:180:A:ALA:H	1:124:A:ASP:HB2	18	0.36
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	1	0.36
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	9	0.36
(1,1547)	1:36:A:LYS:H	1:36:A:LYS:HB2	16	0.36
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	8	0.36
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	14	0.36
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	20	0.36
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	20	0.36
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	11	0.36
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	14	0.36
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	10	0.36
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	2	0.36
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	9	0.36
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	1	0.36
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	6	0.36
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	5	0.36
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	14	0.36
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	7	0.36
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	10	0.36
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	11	0.36
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	20	0.36
(1,1167)	1:179:A:ASN:HB2	1:187:A:VAL:HG21	14	0.36
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	2	0.36
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	19	0.36
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	7	0.36
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	5	0.36
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	12	0.36
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	17	0.36
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	2	0.36
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	8	0.36
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	17	0.36
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	12	0.36
(1,650)	1:86:A:VAL:HG11	1:9:A:LYS:HE2	8	0.36
(1,612)	1:78:A:LEU:HD21	1:106:A:GLN:HG3	17	0.36
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	17	0.36
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	16	0.36
(1,471)	1:47:A:LEU:HB3	1:47:A:LEU:HA	20	0.36
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	3	0.36
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	12	0.36
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	18	0.36
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	16	0.36
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	6	0.36
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	18	0.36
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	19	0.36
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	12	0.36
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	14	0.35
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	3	0.35
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	10	0.35
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	16	0.35
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	9	0.35
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	14	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,322)	1:86:A:VAL:H	1:82:A:ARG:HG2	19	0.35
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	8	0.35
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	8	0.35
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	16	0.35
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	13	0.35
(4,250)	1:77:A:VAL:HB	1:78:A:LEU:HA	14	0.35
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	11	0.35
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	19	0.35
(4,222)	1:67:A:GLU:HG2	1:64:A:GLU:HA	17	0.35
(4,221)	1:178:A:VAL:HB	1:123:A:VAL:HA	18	0.35
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	18	0.35
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	3	0.35
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	6	0.35
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	6	0.35
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	10	0.35
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	3	0.35
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	8	0.35
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	18	0.35
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	16	0.35
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	8	0.35
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	12	0.35
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	15	0.35
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	9	0.35
(1,1774)	1:71:A:LEU:HD21	1:71:A:LEU:H	17	0.35
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	17	0.35
(1,1547)	1:36:A:LYS:H	1:36:A:LYS:HB2	9	0.35
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	4	0.35
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	6	0.35
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	9	0.35
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	12	0.35
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	19	0.35
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	14	0.35
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	4	0.35
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	17	0.35
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	11	0.35
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	12	0.35
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	16	0.35
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	9	0.35
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	4	0.35
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	10	0.35
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	4	0.35
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	17	0.35
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	3	0.35
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	13	0.35
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	8	0.35
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	17	0.35
(1,99)	1:162:A:THR:HG22	1:159:A:TYR:HD1	1	0.35
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	15	0.35
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	6	0.34
(4,380)	1:162:A:THR:H	1:164:A:PRO:HG2	19	0.34
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	6	0.34
(4,369)	1:30:A:CYS:H	1:33:A:ILE:HG13	14	0.34
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	16	0.34
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	3	0.34
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	15	0.34
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	19	0.34
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	8	0.34
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	10	0.34
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	18	0.34
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	6	0.34
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	9	0.34
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	11	0.34
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	12	0.34
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	19	0.34
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	20	0.34
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	2	0.34
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	3	0.34
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	12	0.34
(4,83)	1:8:A:GLU:HA	1:11:A:LYS:HE2	12	0.34
(4,74)	1:10:A:LEU:HD23	1:17:A:PHE:HE1	18	0.34
(4,57)	1:178:A:VAL:HG12	1:178:A:VAL:HB	11	0.34
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	8	0.34
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	3	0.34
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	6	0.34
(1,2461)	1:180:A:ALA:H	1:187:A:VAL:HG21	14	0.34
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	19	0.34
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	20	0.34
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	10	0.34
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	15	0.34
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	15	0.34
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	9	0.34
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	18	0.34
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	7	0.34
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	13	0.34
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	10	0.34
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	5	0.34
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	15	0.34
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD12	19	0.34
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	11	0.34
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	9	0.34
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	10	0.34
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	13	0.34
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	8	0.34
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	13	0.34
(1,741)	1:102:A:ARG:HD2	1:102:A:ARG:HG2	1	0.34
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	15	0.34
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	5	0.34
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	8	0.34
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	1	0.34
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	10	0.34
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	1	0.34
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	16	0.34
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	6	0.34
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	10	0.34
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	20	0.34
(1,339)	1:23:A:GLY:HA3	1:134:A:LEU:HA	8	0.34
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	8	0.34
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	6	0.34
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	13	0.34
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	1	0.34
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	17	0.34
(4,401)	1:24:A:SER:H	1:130:A:MET:HE1	17	0.33
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	1	0.33
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	15	0.33
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	13	0.33
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	12	0.33
(4,347)	1:90:A:ASN:H	1:9:A:LYS:HG2	6	0.33
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	7	0.33
(4,295)	1:46:A:ASP:H	1:47:A:LEU:HB3	5	0.33
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	11	0.33
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	1	0.33
(4,289)	1:158:A:TYR:H	1:160:A:LYS:HE3	12	0.33
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	3	0.33
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	12	0.33
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG22	16	0.33
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	5	0.33
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	16	0.33
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	18	0.33
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	19	0.33
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	20	0.33
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	1	0.33
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	20	0.33
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	6	0.33
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	14	0.33
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	17	0.33
(4,170)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	8	0.33
(4,112)	1:134:A:LEU:HD12	1:137:A:ARG:HD2	19	0.33
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	14	0.33
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	17	0.33
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	2	0.33
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	17	0.33
(4,24)	1:47:A:LEU:HG	1:44:A:THR:HA	20	0.33
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	13	0.33
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	11	0.33
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	11	0.33
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	12	0.33
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	6	0.33
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	10	0.33
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	14	0.33
(1,1858)	1:83:A:ASP:H	1:82:A:ARG:HG2	13	0.33
(1,1790)	1:75:A:GLU:H	1:74:A:LEU:HD11	17	0.33
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	16	0.33
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	20	0.33
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	1	0.33
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	13	0.33
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	13	0.33
(1,1340)	1:37:A:TYR:H	1:33:A:ILE:HG21	1	0.33
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	4	0.33
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	8	0.33
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	13	0.33
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	18	0.33
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	18	0.33
(1,909)	1:136:A:LYS:HA	1:136:A:LYS:HB3	11	0.33
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	9	0.33
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	15	0.33
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	19	0.33
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	4	0.33
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	8	0.33
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	18	0.33
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	13	0.33
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	10	0.33
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	20	0.33
(4,401)	1:24:A:SER:H	1:130:A:MET:HE2	4	0.32
(4,388)	1:138:A:GLY:H	1:135:A:LEU:HB3	11	0.32
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	18	0.32
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	15	0.32
(4,328)	1:153:A:LYS:H	1:152:A:LYS:HA	14	0.32
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	14	0.32
(4,296)	1:46:A:ASP:H	1:47:A:LEU:HD11	17	0.32
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	12	0.32
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	15	0.32
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	4	0.32
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	8	0.32
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	9	0.32
(4,271)	1:64:A:GLU:HB3	1:64:A:GLU:HA	12	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	3	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	4	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	5	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	8	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	13	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	14	0.32
(4,266)	1:128:A:GLU:HB2	1:128:A:GLU:HA	18	0.32
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	9	0.32
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	13	0.32
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	16	0.32
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	18	0.32
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	12	0.32
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	19	0.32
(4,199)	1:8:A:GLU:HG2	1:6:A:MET:H	17	0.32
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	18	0.32
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	10	0.32
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	6	0.32
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	7	0.32
(4,96)	1:76:A:THR:HG22	1:62:A:LEU:HD12	2	0.32
(4,57)	1:18:A:VAL:HG11	1:18:A:VAL:HB	5	0.32
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	1	0.32
(4,28)	1:96:A:LEU:HG	1:198:A:LEU:HG	10	0.32
(4,16)	1:195:A:LEU:HD23	1:198:A:LEU:HB3	17	0.32
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	16	0.32
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	15	0.32
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	11	0.32
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	9	0.32
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	15	0.32
(1,1580)	1:40:A:THR:H	1:39:A:TYR:HB2	18	0.32
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	18	0.32
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	3	0.32
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	19	0.32
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	1	0.32
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	15	0.32
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	20	0.32
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	15	0.32
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	15	0.32
(1,1295)	1:118:A:THR:H	1:15:A:ILE:HD11	12	0.32
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	12	0.32
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	6	0.32
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	19	0.32
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	20	0.32
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	1	0.32
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	13	0.32
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	4	0.32
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	3	0.32
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	13	0.32
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	14	0.32
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	16	0.32
(1,779)	1:109:A:GLU:HA	1:112:A:ARG:HD2	17	0.32
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	13	0.32
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	4	0.32
(1,564)	1:71:A:LEU:HD21	1:71:A:LEU:HB3	20	0.32
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	7	0.32
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	11	0.32
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	9	0.32
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	11	0.32
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	19	0.32
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	18	0.32
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	19	0.32
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	1	0.32
(1,360)	1:31:A:GLU:HG3	1:28:A:THR:HA	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:134:A:LEU:HD11	1:23:A:GLY:HA2	3	0.32
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	2	0.32
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	7	0.32
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	1	0.31
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	14	0.31
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	19	0.31
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	1	0.31
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	15	0.31
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	11	0.31
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	3	0.31
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	4	0.31
(4,243)	1:159:A:TYR:HA	1:163:A:GLU:HG2	19	0.31
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	4	0.31
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	15	0.31
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	11	0.31
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	10	0.31
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	19	0.31
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	5	0.31
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	19	0.31
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	14	0.31
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	20	0.31
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	15	0.31
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	17	0.31
(1,2568)	1:198:A:LEU:H	1:196:A:ASP:HB2	19	0.31
(1,2483)	1:184:A:VAL:H	1:185:A:ASP:HB3	14	0.31
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	10	0.31
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	3	0.31
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	6	0.31
(1,1867)	1:84:A:ALA:H	1:83:A:ASP:HB2	1	0.31
(1,1762)	1:69:A:GLY:H	1:68:A:LYS:HD2	10	0.31
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	2	0.31
(1,1389)	1:9:A:LYS:H	1:9:A:LYS:HD3	12	0.31
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	19	0.31
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	10	0.31
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	5	0.31
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	10	0.31
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	14	0.31
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	6	0.31
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	20	0.31
(1,918)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	17	0.31
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	2	0.31
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	10	0.31
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	19	0.31
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	10	0.31
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	13	0.31
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	6	0.31
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	8	0.31
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	6	0.31
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	15	0.31
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	7	0.31
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	12	0.31
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	13	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE1	3	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	15	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE3	19	0.31
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	20	0.31
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	13	0.31
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	2	0.31
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	4	0.3
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	8	0.3
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	13	0.3
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	18	0.3
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	10	0.3
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	11	0.3
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	2	0.3
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	18	0.3
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	18	0.3
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	11	0.3
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	1	0.3
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	18	0.3
(4,208)	1:156:A:GLU:HG3	1:157:A:THR:HG1	1	0.3
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	5	0.3
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	7	0.3
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	8	0.3
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	12	0.3
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	4	0.3
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	15	0.3
(1,2284)	1:155:A:LEU:H	1:154:A:ARG:HH21	4	0.3
(1,2242)	1:147:A:ASN:H	1:147:A:ASN:HD21	18	0.3
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	13	0.3
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	5	0.3
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	12	0.3
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	14	0.3
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	9	0.3
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	17	0.3
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	18	0.3
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	5	0.3
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	8	0.3
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	17	0.3
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	19	0.3
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	5	0.3
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD12	10	0.3
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	17	0.3
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	2	0.3
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	10	0.3
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	12	0.3
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	17	0.3
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	10	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	1	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	5	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	12	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	15	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	16	0.3
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	20	0.3
(1,833)	1:121:A:LEU:HB3	1:18:A:VAL:HG11	5	0.3
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	7	0.3
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	17	0.3
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	5	0.3
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	20	0.3
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	3	0.3
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	15	0.3
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	15	0.3
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	11	0.3
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	12	0.3
(1,222)	1:105:A:GLN:HA	1:74:A:LEU:HD23	14	0.3
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	7	0.3
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	18	0.3
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG11	20	0.3
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	10	0.29
(4,358)	1:99:A:GLY:H	1:18:A:VAL:HB	12	0.29
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	6	0.29
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	7	0.29
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	9	0.29
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	4	0.29
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	20	0.29
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	9	0.29
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	11	0.29
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	19	0.29
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	6	0.29
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	5	0.29
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	16	0.29
(4,306)	1:143:A:ARG:H	1:138:A:GLY:HA3	5	0.29
(4,301)	1:145:A:ASP:H	1:143:A:ARG:HD2	20	0.29
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	2	0.29
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	19	0.29
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	3	0.29
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	7	0.29
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	10	0.29
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	5	0.29
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	12	0.29
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	2	0.29
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	14	0.29
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	15	0.29
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	4	0.29
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	7	0.29
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	20	0.29
(4,83)	1:64:A:GLU:HA	1:68:A:LYS:HE3	8	0.29
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	3	0.29
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	7	0.29
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	11	0.29
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	12	0.29
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	19	0.29
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	13	0.29
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	4	0.29
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	6	0.29
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	8	0.29
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	17	0.29
(1,1785)	1:74:A:LEU:H	1:75:A:GLU:HG2	20	0.29
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	4	0.29
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	9	0.29
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	16	0.29
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	17	0.29
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	1	0.29
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	15	0.29
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	3	0.29
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	8	0.29
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	15	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	1	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	2	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	3	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	7	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	10	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	11	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	12	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	14	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	15	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	16	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	19	0.29
(1,946)	1:146:A:ASP:HA	1:146:A:ASP:HB2	20	0.29
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	6	0.29
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	7	0.29
(1,835)	1:123:A:VAL:HG21	1:121:A:LEU:HB2	19	0.29
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	18	0.29
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	20	0.29
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	20	0.29
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	8	0.29
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	10	0.29
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	15	0.29
(1,564)	1:71:A:LEU:HD21	1:71:A:LEU:HB3	6	0.29
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	1	0.29
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	8	0.29
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	2	0.29
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	3	0.29
(1,507)	1:58:A:ARG:HB2	1:58:A:ARG:HD3	10	0.29
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	17	0.29
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	3	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	1	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	5	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	7	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	8	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	10	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	12	0.29
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	17	0.29
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	3	0.29
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	14	0.29
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE2	8	0.29
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	4	0.29
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG23	2	0.29
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	3	0.28
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	7	0.28
(4,344)	1:39:A:TYR:H	1:34:A:VAL:HG11	1	0.28
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	3	0.28
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	8	0.28
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	8	0.28
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	10	0.28
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	2	0.28
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	14	0.28
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	15	0.28
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	17	0.28
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	10	0.28
(4,217)	1:47:A:LEU:HD13	1:43:A:SER:HB3	5	0.28
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	16	0.28
(4,158)	1:97:A:ILE:HG22	1:43:A:SER:HB2	2	0.28
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	6	0.28
(4,82)	1:10:A:LEU:HD22	1:89:A:VAL:HB	17	0.28
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	16	0.28
(1,2467)	1:182:A:GLY:H	1:133:A:ARG:HH11	3	0.28
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	12	0.28
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	13	0.28
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	17	0.28
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	8	0.28
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	13	0.28
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	7	0.28
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	18	0.28
(1,2086)	1:116:A:GLN:H	1:115:A:GLY:HA2	2	0.28
(1,1993)	1:102:A:ARG:H	1:102:A:ARG:HD2	4	0.28
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	5	0.28
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	8	0.28
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	2	0.28
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	16	0.28
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	16	0.28
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	15	0.28
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	3	0.28
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	16	0.28
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	1	0.28
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	19	0.28
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	3	0.28
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	17	0.28
(1,1121)	1:174:A:ILE:HD11	1:117:A:PRO:HD2	1	0.28
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	3	0.28
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	10	0.28
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	20	0.28
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	11	0.28
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	3	0.28
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	19	0.28
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	8	0.28
(1,782)	1:112:A:ARG:HB2	1:113:A:ARG:HD2	2	0.28
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	5	0.28
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	6	0.28
(1,564)	1:71:A:LEU:HD21	1:71:A:LEU:HB3	16	0.28
(1,564)	1:71:A:LEU:HD21	1:71:A:LEU:HB3	19	0.28
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	17	0.28
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	15	0.28
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	2	0.28
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	20	0.28
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	12	0.28
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	5	0.28
(1,339)	1:23:A:GLY:HA3	1:134:A:LEU:HA	3	0.28
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	9	0.28
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	16	0.28
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	18	0.28
(1,235)	1:9:A:LYS:HG3	1:9:A:LYS:HA	16	0.28
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	5	0.28
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	16	0.28
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG23	10	0.28
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG23	16	0.28
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	9	0.27
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	1	0.27
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	8	0.27
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	18	0.27
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	20	0.27
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	18	0.27
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	3	0.27
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	11	0.27
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	20	0.27
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	15	0.27
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	19	0.27
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	2	0.27
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	10	0.27
(4,243)	1:159:A:TYR:HA	1:163:A:GLU:HG3	7	0.27
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	6	0.27
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	13	0.27
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	18	0.27
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	15	0.27
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	15	0.27
(4,196)	1:131:A:THR:HA	1:134:A:LEU:HG	1	0.27
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	13	0.27
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	3	0.27
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	9	0.27
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	18	0.27
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	8	0.27
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	10	0.27
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	13	0.27
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	19	0.27
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	18	0.27
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	5	0.27
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	11	0.27
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	3	0.27
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	11	0.27
(1,2215)	1:143:A:ARG:H	1:143:A:ARG:HB3	3	0.27
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	8	0.27
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	9	0.27
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	14	0.27
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	1	0.27
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	12	0.27
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	13	0.27
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	19	0.27
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	11	0.27
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	6	0.27
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	19	0.27
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	11	0.27
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	18	0.27
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	7	0.27
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	5	0.27
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	11	0.27
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	18	0.27
(1,1329)	1:43:A:SER:H	1:42:A:LEU:HD12	16	0.27
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	3	0.27
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	7	0.27
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	10	0.27
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	16	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	1	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	2	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	3	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	4	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	5	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	6	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	8	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	9	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	12	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	13	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	14	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	17	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	18	0.27
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	20	0.27
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	16	0.27
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	6	0.27
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	15	0.27
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	16	0.27
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	12	0.27
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	13	0.27
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	18	0.27
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	20	0.27
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	19	0.27
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	10	0.27
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	9	0.27
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	6	0.27
(1,605)	1:78:A:LEU:HA	1:113:A:ARG:HD2	8	0.27
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	9	0.27
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	15	0.27
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	15	0.27
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	14	0.27
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	7	0.27
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	19	0.27
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	5	0.27
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	20	0.27
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	8	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	4	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	6	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	8	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	9	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	12	0.27
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	13	0.27
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	13	0.27
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG23	8	0.27
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	12	0.26
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	12	0.26
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	13	0.26
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	14	0.26
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	2	0.26
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	15	0.26
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	16	0.26
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	5	0.26
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	18	0.26
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	12	0.26
(4,328)	1:153:A:LYS:H	1:152:A:LYS:HA	13	0.26
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	13	0.26
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	5	0.26
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	6	0.26
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG22	2	0.26
(4,249)	1:18:A:VAL:HA	1:19:A:VAL:HG21	5	0.26
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	15	0.26
(4,243)	1:159:A:TYR:HA	1:163:A:GLU:HG3	8	0.26
(4,196)	1:131:A:THR:HA	1:134:A:LEU:HG	16	0.26
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	1	0.26
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	18	0.26
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	10	0.26
(4,144)	1:89:A:VAL:HG23	1:6:A:MET:H	5	0.26
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	10	0.26
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	8	0.26
(4,94)	1:76:A:THR:HG21	1:75:A:GLU:HB2	10	0.26
(4,83)	1:105:A:GLN:HA	1:105:A:GLN:HG2	9	0.26
(4,81)	1:10:A:LEU:HD22	1:85:A:MET:HA	8	0.26
(4,79)	1:191:A:VAL:HG12	1:178:A:VAL:HG23	11	0.26
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	6	0.26
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	3	0.26
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	18	0.26
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	2	0.26
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	16	0.26
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	15	0.26
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	19	0.26
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	20	0.26
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	20	0.26
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	1	0.26
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	11	0.26
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	13	0.26
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	6	0.26
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	3	0.26
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	6	0.26
(1,1871)	1:84:A:ALA:H	1:85:A:MET:HG3	4	0.26
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	1	0.26
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	2	0.26
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	4	0.26
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	5	0.26
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	9	0.26
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	10	0.26
(1,1647)	1:50:A:SER:H	1:51:A:GLU:HB3	15	0.26
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	3	0.26
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	10	0.26
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	13	0.26
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	14	0.26
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	7	0.26
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	8	0.26
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	19	0.26
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	17	0.26
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	4	0.26
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	11	0.26
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	15	0.26
(1,1320)	1:12:A:LYS:H	1:12:A:LYS:HD2	14	0.26
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	8	0.26
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	14	0.26
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	8	0.26
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	3	0.26
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	2	0.26
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	8	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	7	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	10	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	11	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	15	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	16	0.26
(1,1101)	1:168:A:PHE:HB2	1:168:A:PHE:HZ	19	0.26
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	5	0.26
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	13	0.26
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	4	0.26
(1,807)	1:116:A:GLN:HG2	1:111:A:GLU:HA	17	0.26
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	16	0.26
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	5	0.26
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	19	0.26
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	14	0.26
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	2	0.26
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	4	0.26
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	7	0.26
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	15	0.26
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	14	0.26
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	19	0.26
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	7	0.26
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	18	0.26
(1,480)	1:48:A:LEU:HB2	1:48:A:LEU:HD11	10	0.26
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	3	0.26
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	17	0.26
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	2	0.26
(1,447)	1:43:A:SER:HA	1:98:A:ASP:HB2	1	0.26
(1,343)	1:24:A:SER:HA	1:130:A:MET:HB2	11	0.26
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	11	0.26
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	19	0.26
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	20	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	1	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	5	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	11	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	15	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	16	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	17	0.26
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	19	0.26
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	1	0.26
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	10	0.26
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	6	0.26
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	10	0.25
(4,382)	1:21:A:GLY:H	1:26:A:LYS:HE3	6	0.25
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	1	0.25
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG23	10	0.25
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	18	0.25
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	20	0.25
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	11	0.25
(4,341)	1:80:A:MET:H	1:80:A:MET:HE3	7	0.25
(4,335)	1:52:A:VAL:H	1:62:A:LEU:HD13	9	0.25
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	17	0.25
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	6	0.25
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	17	0.25
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	1	0.25
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	11	0.25
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	5	0.25
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	7	0.25
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	11	0.25
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	12	0.25
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	18	0.25
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	7	0.25
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	13	0.25
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	14	0.25
(4,258)	1:72:A:VAL:HA	1:62:A:LEU:HB3	4	0.25
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	3	0.25
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	3	0.25
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	20	0.25
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	1	0.25
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	16	0.25
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	20	0.25
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	3	0.25
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	16	0.25
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	5	0.25
(4,33)	1:164:A:PRO:HG2	1:162:A:THR:HA	6	0.25
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	20	0.25
(4,3)	1:10:A:LEU:HD13	1:13:A:THR:HA	12	0.25
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	12	0.25
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	10	0.25
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	19	0.25
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	15	0.25
(1,2158)	1:128:A:GLU:H	1:128:A:GLU:HB2	19	0.25
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	19	0.25
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	13	0.25
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	16	0.25
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	5	0.25
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	8	0.25
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	11	0.25
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	3	0.25
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	6	0.25
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	14	0.25
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	11	0.25
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	18	0.25
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	5	0.25
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	8	0.25
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	11	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	6	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	7	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	8	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	9	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	15	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	16	0.25
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	19	0.25
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	12	0.25
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	14	0.25
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	3	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	6	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	7	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	10	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	11	0.25
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	13	0.25
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	12	0.25
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	7	0.25
(1,1361)	1:112:A:ARG:H	1:114:A:ILE:HD11	1	0.25
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	11	0.25
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	12	0.25
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	11	0.25
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	17	0.25
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	7	0.25
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	16	0.25
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	7	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	1	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	2	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	3	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	6	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	8	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	11	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	12	0.25
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	13	0.25
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	5	0.25
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	20	0.25
(1,995)	1:152:A:LYS:HA	1:152:A:LYS:HD2	13	0.25
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	3	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	1	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	2	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	6	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	7	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	8	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	10	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	11	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	15	0.25
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	17	0.25
(1,877)	1:128:A:GLU:HB2	1:127:A:PRO:HD2	19	0.25
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	19	0.25
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	17	0.25
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	15	0.25
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	20	0.25
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	1	0.25
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	6	0.25
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	2	0.25
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	10	0.25
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	7	0.25
(1,474)	1:47:A:LEU:HD11	1:46:A:ASP:HB2	17	0.25
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	4	0.25
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	6	0.25
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	8	0.25
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	9	0.25
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	15	0.25
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	9	0.25
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	13	0.25
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	1	0.25
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	9	0.25
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	8	0.25
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	9	0.25
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	2	0.25
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	18	0.25
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	7	0.25
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	2	0.25
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	12	0.25
(1,56)	1:78:A:LEU:HD22	1:77:A:VAL:HG12	16	0.25
(1,26)	1:74:A:LEU:HG	1:106:A:GLN:HG2	15	0.25
(4,401)	1:24:A:SER:H	1:130:A:MET:HE2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	7	0.24
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	9	0.24
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	13	0.24
(4,370)	1:50:A:SER:H	1:80:A:MET:HE2	10	0.24
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	8	0.24
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	8	0.24
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	11	0.24
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	4	0.24
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	5	0.24
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	6	0.24
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	14	0.24
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	3	0.24
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	11	0.24
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	2	0.24
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	7	0.24
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	14	0.24
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	10	0.24
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	10	0.24
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	17	0.24
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	8	0.24
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	13	0.24
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	17	0.24
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	3	0.24
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	7	0.24
(4,286)	1:163:A:GLU:H	1:160:A:LYS:HE2	16	0.24
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	9	0.24
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	17	0.24
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	20	0.24
(4,237)	1:60:A:LYS:HB3	1:57:A:ALA:HA	5	0.24
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	6	0.24
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	8	0.24
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HB2	7	0.24
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	17	0.24
(4,96)	1:76:A:THR:HG22	1:62:A:LEU:HD12	15	0.24
(4,88)	1:76:A:THR:HG23	1:73:A:PRO:HB3	17	0.24
(4,82)	1:10:A:LEU:HD21	1:116:A:GLN:HG2	14	0.24
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	11	0.24
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	1	0.24
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	3	0.24
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	6	0.24
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	7	0.24
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	12	0.24
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	14	0.24
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	19	0.24
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	20	0.24
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	16	0.24
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	15	0.24
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	11	0.24
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	20	0.24
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	2	0.24
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	18	0.24
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	19	0.24
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	3	0.24
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	11	0.24
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	14	0.24
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	13	0.24
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	8	0.24
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	14	0.24
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	11	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	1	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	2	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	4	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	5	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	17	0.24
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	20	0.24
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	1	0.24
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	20	0.24
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	10	0.24
(1,1416)	1:14:A:LYS:H	1:14:A:LYS:HG2	13	0.24
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	13	0.24
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	8	0.24
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	15	0.24
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	9	0.24
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	7	0.24
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	6	0.24
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	4	0.24
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	11	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	4	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	5	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	9	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	10	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	15	0.24
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	4	0.24
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	9	0.24
(1,1148)	1:177:A:LYS:HG3	1:122:A:TYR:HD1	14	0.24
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	16	0.24
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	7	0.24
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	4	0.24
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	5	0.24
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	10	0.24
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	16	0.24
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	5	0.24
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	9	0.24
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	14	0.24
(1,923)	1:139:A:GLU:HG3	1:139:A:GLU:HA	16	0.24
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	16	0.24
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	18	0.24
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	19	0.24
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	11	0.24
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	12	0.24
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	2	0.24
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	5	0.24
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	16	0.24
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	16	0.24
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	18	0.24
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	3	0.24
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	3	0.24
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	9	0.24
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	14	0.24
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	20	0.24
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	9	0.24
(1,451)	1:43:A:SER:HB2	1:44:A:THR:HG21	15	0.24
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	11	0.24
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	16	0.24
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	3	0.24
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	4	0.24
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	6	0.24
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	17	0.24
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	5	0.24
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	5	0.24
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	4	0.24
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	2	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	3	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	6	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	7	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	9	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	10	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	12	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	13	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	14	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	15	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	17	0.24
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	20	0.24
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	7	0.24
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	10	0.24
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	20	0.24
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	5	0.24
(1,81)	1:76:A:THR:HG22	1:58:A:ARG:HD2	20	0.24
(1,61)	1:118:A:THR:HG22	1:15:A:ILE:HB	18	0.24
(4,401)	1:24:A:SER:H	1:130:A:MET:HE3	19	0.23
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	20	0.23
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	4	0.23
(4,359)	1:169:A:TYR:H	1:171:A:LYS:HB2	19	0.23
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	4	0.23
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	13	0.23
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	1	0.23
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	18	0.23
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HB3	3	0.23
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	6	0.23
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	9	0.23
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	14	0.23
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	5	0.23
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	10	0.23
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	15	0.23
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	19	0.23
(4,243)	1:189:A:SER:HA	1:192:A:CYS:HB3	15	0.23
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	2	0.23
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	16	0.23
(4,211)	1:139:A:GLU:HG2	1:136:A:LYS:HE2	14	0.23
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	4	0.23
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	11	0.23
(4,167)	1:174:A:ILE:HD12	1:174:A:ILE:HG23	13	0.23
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	11	0.23
(4,92)	1:76:A:THR:HG22	1:80:A:MET:HG3	7	0.23
(4,50)	1:88:A:LYS:HG3	1:88:A:LYS:HE2	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:68:A:LYS:HD2	1:64:A:GLU:HA	14	0.23
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	4	0.23
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	8	0.23
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	10	0.23
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	16	0.23
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	5	0.23
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	17	0.23
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	20	0.23
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	4	0.23
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	7	0.23
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	16	0.23
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	10	0.23
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	17	0.23
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	9	0.23
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	17	0.23
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	20	0.23
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	18	0.23
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	19	0.23
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	4	0.23
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	6	0.23
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	16	0.23
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	11	0.23
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	17	0.23
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	7	0.23
(1,1584)	1:40:A:THR:HG21	1:40:A:THR:H	12	0.23
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	3	0.23
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	15	0.23
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	6	0.23
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	10	0.23
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	18	0.23
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	9	0.23
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	17	0.23
(1,1381)	1:7:A:GLU:H	1:82:A:ARG:HH11	15	0.23
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	1	0.23
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	18	0.23
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	13	0.23
(1,1272)	1:47:A:LEU:H	1:46:A:ASP:HB2	14	0.23
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	5	0.23
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	14	0.23
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	2	0.23
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	16	0.23
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	19	0.23
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	17	0.23
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	19	0.23
(1,1026)	1:160:A:LYS:HG3	1:160:A:LYS:HA	13	0.23
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	14	0.23
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	17	0.23
(1,984)	1:148:A:GLU:HG3	1:151:A:ILE:HG13	2	0.23
(1,960)	1:149:A:GLU:HG2	1:153:A:LYS:HB3	20	0.23
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	1	0.23
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	15	0.23
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	14	0.23
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	14	0.23
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	13	0.23
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	8	0.23
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	7	0.23
(1,648)	1:86:A:VAL:HG11	1:6:A:MET:HG2	12	0.23
(1,605)	1:78:A:LEU:HA	1:113:A:ARG:HD2	9	0.23
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	5	0.23
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	14	0.23
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	16	0.23
(1,511)	1:58:A:ARG:HD2	1:59:A:GLY:HA2	13	0.23
(1,426)	1:40:A:THR:HG21	1:88:A:LYS:HB3	17	0.23
(1,341)	1:134:A:LEU:HD11	1:23:A:GLY:HA2	17	0.23
(1,337)	1:23:A:GLY:HA2	1:133:A:ARG:HD3	15	0.23
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	7	0.23
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	14	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	1	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	5	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	8	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	11	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	16	0.23
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	19	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	1	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	3	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	4	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	5	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	6	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	8	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	9	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	13	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	15	0.23
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	14	0.23
(1,188)	1:85:A:MET:HA	1:40:A:THR:HG21	14	0.23
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG12	10	0.23
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	3	0.23
(1,77)	1:34:A:VAL:HG11	1:41:A:HIS:HB3	14	0.23
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	9	0.23
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	16	0.23
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	2	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	6	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	11	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	14	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	19	0.22
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	16	0.22
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	10	0.22
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	9	0.22
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	16	0.22
(4,347)	1:90:A:ASN:H	1:9:A:LYS:HG2	7	0.22
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	17	0.22
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	20	0.22
(4,321)	1:86:A:VAL:H	1:6:A:MET:HB3	10	0.22
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	4	0.22
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	10	0.22
(4,298)	1:81:A:LEU:H	1:47:A:LEU:HB3	3	0.22
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	18	0.22
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	3	0.22
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	7	0.22
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	18	0.22
(4,283)	1:151:A:ILE:H	1:145:A:ASP:HB3	20	0.22
(4,271)	1:67:A:GLU:HB2	1:64:A:GLU:HA	15	0.22
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	5	0.22
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	6	0.22
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	15	0.22
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	9	0.22
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	7	0.22
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	14	0.22
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	18	0.22
(4,107)	1:129:A:THR:HG23	1:181:A:GLU:HG2	11	0.22
(4,101)	1:191:A:VAL:HG22	1:191:A:VAL:HA	2	0.22
(4,101)	1:191:A:VAL:HG22	1:191:A:VAL:HA	8	0.22
(4,101)	1:191:A:VAL:HG22	1:191:A:VAL:HA	14	0.22
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	3	0.22
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	1:76:A:THR:HG21	1:73:A:PRO:HG3	12	0.22
(4,82)	1:10:A:LEU:HD21	1:116:A:GLN:HG2	6	0.22
(4,72)	1:103:A:GLU:HA	1:103:A:GLU:HG3	9	0.22
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	15	0.22
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	3	0.22
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	9	0.22
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	9	0.22
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	10	0.22
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	18	0.22
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	3	0.22
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	6	0.22
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	13	0.22
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	15	0.22
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	17	0.22
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	3	0.22
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	5	0.22
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	18	0.22
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	11	0.22
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	2	0.22
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	15	0.22
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	15	0.22
(1,2024)	1:106:A:GLN:H	1:105:A:GLN:HB3	15	0.22
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	14	0.22
(1,1993)	1:102:A:ARG:H	1:102:A:ARG:HD2	14	0.22
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	18	0.22
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	20	0.22
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	16	0.22
(1,1638)	1:49:A:ARG:H	1:46:A:ASP:HB2	20	0.22
(1,1621)	1:45:A:GLY:H	1:47:A:LEU:HB2	20	0.22
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	10	0.22
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	18	0.22
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	1	0.22
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	11	0.22
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	6	0.22
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	13	0.22
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	8	0.22
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	8	0.22
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	18	0.22
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	19	0.22
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	3	0.22
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	8	0.22
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG21	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	1	0.22
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	8	0.22
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	16	0.22
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	18	0.22
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	11	0.22
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	20	0.22
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	7	0.22
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	17	0.22
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	15	0.22
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	6	0.22
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	13	0.22
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	3	0.22
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	12	0.22
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	5	0.22
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	1	0.22
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	2	0.22
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	17	0.22
(1,813)	1:118:A:THR:HG21	1:14:A:LYS:HE2	19	0.22
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	2	0.22
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	9	0.22
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	2	0.22
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	3	0.22
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	12	0.22
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	19	0.22
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	2	0.22
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	16	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	9	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	11	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	12	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	17	0.22
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	20	0.22
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	5	0.22
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	10	0.22
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	14	0.22
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	5	0.22
(1,637)	1:84:A:ALA:HA	1:83:A:ASP:HB2	20	0.22
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	20	0.22
(1,605)	1:78:A:LEU:HA	1:113:A:ARG:HD2	10	0.22
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	12	0.22
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	13	0.22
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	11	0.22
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	14	0.22
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	16	0.22
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	19	0.22
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	17	0.22
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	11	0.22
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	12	0.22
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	16	0.22
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	19	0.22
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	2	0.22
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	2	0.22
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	12	0.22
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	1	0.22
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	16	0.22
(1,331)	1:22:A:PRO:HA	1:26:A:LYS:HB2	16	0.22
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	2	0.22
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	13	0.22
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	2	0.22
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	20	0.22
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	8	0.22
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	20	0.22
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	2	0.22
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	14	0.22
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE1	10	0.22
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	14	0.22
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	2	0.22
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	14	0.22
(1,104)	1:184:A:VAL:HG21	1:184:A:VAL:HB	18	0.22
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	12	0.22
(1,91)	1:134:A:LEU:HD13	1:135:A:LEU:HA	8	0.22
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	6	0.22
(1,48)	1:81:A:LEU:HD11	1:42:A:LEU:HA	12	0.22
(1,34)	1:106:A:GLN:HB2	1:101:A:PRO:HB3	13	0.22
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	5	0.22
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	3	0.21
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	9	0.21
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	13	0.21
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	18	0.21
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	17	0.21
(4,340)	1:80:A:MET:H	1:76:A:THR:HG22	14	0.21
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	9	0.21
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	12	0.21
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	9	0.21
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	13	0.21
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	15	0.21
(4,306)	1:139:A:GLU:H	1:138:A:GLY:HA3	9	0.21
(4,305)	1:155:A:LEU:H	1:156:A:GLU:HG2	2	0.21
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	19	0.21
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	13	0.21
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	3	0.21
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	8	0.21
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	9	0.21
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	13	0.21
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	17	0.21
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	11	0.21
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	1	0.21
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	2	0.21
(4,126)	1:144:A:VAL:HG11	1:70:A:GLN:HB2	9	0.21
(4,101)	1:178:A:VAL:HG13	1:123:A:VAL:HA	15	0.21
(4,95)	1:76:A:THR:HG23	1:58:A:ARG:HG2	11	0.21
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	20	0.21
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	2	0.21
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	15	0.21
(1,2432)	1:178:A:VAL:H	1:177:A:LYS:HB2	18	0.21
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	3	0.21
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	6	0.21
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	13	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	1	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	7	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	9	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	12	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	14	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	19	0.21
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	20	0.21
(1,2388)	1:173:A:GLY:H	1:169:A:TYR:HB2	17	0.21
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	7	0.21
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	19	0.21
(1,2238)	1:146:A:ASP:H	1:147:A:ASN:HD22	18	0.21
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	1	0.21
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	4	0.21
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	14	0.21
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	4	0.21
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	4	0.21
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	16	0.21
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	4	0.21
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	11	0.21
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	15	0.21
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	17	0.21
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	18	0.21
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	19	0.21
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	3	0.21
(1,1928)	1:92:A:SER:H	1:88:A:LYS:HG2	18	0.21
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	18	0.21
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	11	0.21
(1,1690)	1:58:A:ARG:H	1:58:A:ARG:HE	14	0.21
(1,1688)	1:58:A:ARG:H	1:58:A:ARG:HB3	3	0.21
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	1	0.21
(1,1609)	1:43:A:SER:H	1:46:A:ASP:HB2	14	0.21
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	11	0.21
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	13	0.21
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	18	0.21
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	2	0.21
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	4	0.21
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	14	0.21
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	3	0.21
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	11	0.21
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	14	0.21
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	15	0.21
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	18	0.21
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	13	0.21
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	19	0.21
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	19	0.21
(1,1203)	1:190:A:GLN:HA	1:190:A:GLN:HG3	20	0.21
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	13	0.21
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	15	0.21
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	20	0.21
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	6	0.21
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	15	0.21
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	13	0.21
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	1	0.21
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	4	0.21
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	17	0.21
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	3	0.21
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	6	0.21
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	13	0.21
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	4	0.21
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	4	0.21
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	5	0.21
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	6	0.21
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	7	0.21
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	4	0.21
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	14	0.21
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	19	0.21
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	11	0.21
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	3	0.21
(1,653)	1:87:A:ALA:HB1	1:83:A:ASP:HB2	3	0.21
(1,595)	1:77:A:VAL:HB	1:74:A:LEU:HA	5	0.21
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	4	0.21
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	6	0.21
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	20	0.21
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	3	0.21
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	9	0.21
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	2	0.21
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	5	0.21
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	6	0.21
(1,468)	1:48:A:LEU:HD11	1:45:A:GLY:HA2	5	0.21
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	11	0.21
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	13	0.21
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	17	0.21
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	11	0.21
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	13	0.21
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	4	0.21
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	5	0.21
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	16	0.21
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	20	0.21
(1,268)	1:14:A:LYS:HB2	1:199:A:LYS:HA	11	0.21
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	13	0.21
(1,229)	1:7:A:GLU:HB3	1:7:A:GLU:HG3	18	0.21
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	16	0.21
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	6	0.21
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	11	0.21
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	16	0.21
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	7	0.21
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	11	0.21
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	20	0.21
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	8	0.2
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	18	0.2
(4,374)	1:150:A:THR:H	1:147:A:ASN:HB2	13	0.2
(4,369)	1:30:A:CYS:H	1:191:A:VAL:HG21	13	0.2
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	17	0.2
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	19	0.2
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	11	0.2
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	12	0.2
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	6	0.2
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	17	0.2
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	15	0.2
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	16	0.2
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	20	0.2
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	4	0.2
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	14	0.2
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	16	0.2
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	2	0.2
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	13	0.2
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	8	0.2
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	17	0.2
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	11	0.2
(4,210)	1:170:A:GLU:HG2	1:170:A:GLU:HA	8	0.2
(4,210)	1:170:A:GLU:HG2	1:170:A:GLU:HA	17	0.2
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	20	0.2
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	20	0.2
(4,97)	1:44:A:THR:HG22	1:100:A:TYR:HA	5	0.2
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	14	0.2
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	1	0.2
(4,24)	1:106:A:GLN:HB3	1:101:A:PRO:HD2	10	0.2
(1,2463)	1:181:A:GLU:H	1:179:A:ASN:HB2	14	0.2
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	2	0.2
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	5	0.2
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	18	0.2
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	12	0.2
(1,2269)	1:152:A:LYS:H	1:152:A:LYS:HB3	13	0.2
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	11	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	1	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	3	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	5	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	6	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	9	0.2
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	13	0.2
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	16	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	3	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	6	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	7	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	8	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	14	0.2
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	17	0.2
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	16	0.2
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	20	0.2
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	4	0.2
(1,1773)	1:71:A:LEU:H	1:71:A:LEU:HB3	4	0.2
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	3	0.2
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	10	0.2
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	8	0.2
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	17	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	1	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	3	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	6	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	10	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	14	0.2
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	20	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	5	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	10	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	12	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	13	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	18	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	19	0.2
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	20	0.2
(1,1508)	1:30:A:CYS:H	1:27:A:GLY:H	18	0.2
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	3	0.2
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	5	0.2
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	17	0.2
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	3	0.2
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	15	0.2
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	11	0.2
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	16	0.2
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	18	0.2
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	8	0.2
(1,1255)	1:100:A:TYR:H	1:44:A:THR:HG23	16	0.2
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	2	0.2
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	12	0.2
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	16	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	1	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	3	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	7	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	10	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	12	0.2
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	14	0.2
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	13	0.2
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	18	0.2
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	20	0.2
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	3	0.2
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	11	0.2
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	3	0.2
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	8	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	2	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	3	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	8	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	9	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	11	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	13	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	16	0.2
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	17	0.2
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	7	0.2
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	8	0.2
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	20	0.2
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	1	0.2
(1,776)	1:111:A:GLU:HG3	1:116:A:GLN:HA	1	0.2
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	5	0.2
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	6	0.2
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	7	0.2
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	4	0.2
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	12	0.2
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	3	0.2
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	6	0.2
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	3	0.2
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	14	0.2
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	19	0.2
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	6	0.2
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	9	0.2
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	10	0.2
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	2	0.2
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	11	0.2
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	18	0.2
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	3	0.2
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	5	0.2
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	6	0.2
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	7	0.2
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	8	0.2
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	19	0.2
(1,533)	1:64:A:GLU:HG2	1:65:A:ILE:HA	15	0.2
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	1	0.2
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	12	0.2
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	20	0.2
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	6	0.2
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	9	0.2
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	10	0.2
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	13	0.2
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	20	0.2
(1,467)	1:44:A:THR:HG21	1:100:A:TYR:HE1	15	0.2
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	4	0.2
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	5	0.2
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	12	0.2
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	3	0.2
(1,343)	1:24:A:SER:HA	1:130:A:MET:HB2	14	0.2
(1,336)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	17	0.2
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	1	0.2
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	12	0.2
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	11	0.2
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	14	0.2
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	18	0.2
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	11	0.2
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	1	0.2
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	17	0.2
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	17	0.2
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	15	0.2
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	4	0.2
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	5	0.2
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	6	0.2
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	12	0.2
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	18	0.2
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	16	0.19
(4,394)	1:186:A:SER:H	1:186:A:SER:HB2	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	11	0.19
(4,380)	1:162:A:THR:H	1:160:A:LYS:HB2	17	0.19
(4,379)	1:37:A:TYR:H	1:36:A:LYS:HG2	2	0.19
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	15	0.19
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	5	0.19
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	14	0.19
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	18	0.19
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	15	0.19
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	9	0.19
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	18	0.19
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	20	0.19
(4,305)	1:155:A:LEU:H	1:156:A:GLU:HG2	14	0.19
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	2	0.19
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	1	0.19
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	7	0.19
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	20	0.19
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	8	0.19
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	9	0.19
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	12	0.19
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	6	0.19
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	7	0.19
(4,163)	1:166:A:ILE:HG21	1:170:A:GLU:HA	10	0.19
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	9	0.19
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	13	0.19
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	2	0.19
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	13	0.19
(4,80)	1:78:A:LEU:HD22	1:81:A:LEU:HD23	12	0.19
(4,50)	1:88:A:LYS:HG3	1:88:A:LYS:HE2	17	0.19
(4,44)	1:160:A:LYS:HA	1:160:A:LYS:HE3	8	0.19
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	1	0.19
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	11	0.19
(4,20)	1:74:A:LEU:HG	1:105:A:GLN:HB2	15	0.19
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	13	0.19
(1,2429)	1:178:A:VAL:H	1:122:A:TYR:HD2	2	0.19
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	11	0.19
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	14	0.19
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	4	0.19
(1,2221)	1:144:A:VAL:H	1:143:A:ARG:HD2	9	0.19
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	3	0.19
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	13	0.19
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	11	0.19
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	12	0.19
(1,2136)	1:124:A:ASP:H	1:122:A:TYR:HB2	8	0.19
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	16	0.19
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	18	0.19
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	19	0.19
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	14	0.19
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	5	0.19
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	12	0.19
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	17	0.19
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	2	0.19
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	3	0.19
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	19	0.19
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	2	0.19
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	10	0.19
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	5	0.19
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	14	0.19
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	15	0.19
(1,1814)	1:77:A:VAL:H	1:78:A:LEU:HG	16	0.19
(1,1690)	1:58:A:ARG:H	1:58:A:ARG:HE	17	0.19
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	3	0.19
(1,1652)	1:51:A:GLU:H	1:51:A:GLU:HG3	14	0.19
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	19	0.19
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	2	0.19
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	20	0.19
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	5	0.19
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	6	0.19
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	11	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	2	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	4	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	5	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	7	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	8	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	9	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	15	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	16	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	17	0.19
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	19	0.19
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	6	0.19
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	7	0.19
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	8	0.19
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	17	0.19
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	19	0.19
(1,1416)	1:14:A:LYS:H	1:14:A:LYS:HG2	15	0.19
(1,1407)	1:13:A:THR:H	1:12:A:LYS:HB3	2	0.19
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	2	0.19
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG12	6	0.19
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	6	0.19
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	15	0.19
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	17	0.19
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	18	0.19
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	4	0.19
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	11	0.19
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	1	0.19
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	3	0.19
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	2	0.19
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	5	0.19
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	9	0.19
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	18	0.19
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	1	0.19
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	2	0.19
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	7	0.19
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	10	0.19
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	16	0.19
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	10	0.19
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	7	0.19
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	12	0.19
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	18	0.19
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	18	0.19
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	13	0.19
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	13	0.19
(1,955)	1:148:A:GLU:HA	1:148:A:GLU:HG3	20	0.19
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	5	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	1	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	4	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	10	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	12	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	14	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	15	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	18	0.19
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	20	0.19
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	3	0.19
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	12	0.19
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	16	0.19
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	5	0.19
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	7	0.19
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	11	0.19
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	4	0.19
(1,777)	1:111:A:GLU:HG2	1:116:A:GLN:HG2	11	0.19
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	8	0.19
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	2	0.19
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	5	0.19
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	13	0.19
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	18	0.19
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	20	0.19
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	1	0.19
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	7	0.19
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	16	0.19
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	5	0.19
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	6	0.19
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	14	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	2	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	3	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	7	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	15	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	16	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	18	0.19
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	20	0.19
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	3	0.19
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	17	0.19
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	4	0.19
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	9	0.19
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	14	0.19
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	3	0.19
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	20	0.19
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	18	0.19
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	8	0.19
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	17	0.19
(1,587)	1:75:A:GLU:HA	1:74:A:LEU:HD11	16	0.19
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	7	0.19
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	10	0.19
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	12	0.19
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	20	0.19
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	18	0.19
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	3	0.19
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	17	0.19
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	18	0.19
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	19	0.19
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	3	0.19
(1,408)	1:36:A:LYS:HE3	1:36:A:LYS:HB3	9	0.19
(1,364)	1:28:A:THR:HG21	1:32:A:LYS:HG2	16	0.19
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	8	0.19
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	11	0.19
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	11	0.19
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	8	0.19
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	12	0.19
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	16	0.19
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	6	0.19
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	15	0.19
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	16	0.19
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	19	0.19
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	4	0.19
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	10	0.19
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	18	0.19
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	10	0.19
(1,108)	1:34:A:VAL:HG23	1:40:A:THR:HA	15	0.19
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	6	0.19
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	18	0.19
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	19	0.19
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	2	0.19
(1,89)	1:191:A:VAL:HG23	1:195:A:LEU:HD22	18	0.19
(1,77)	1:34:A:VAL:HG12	1:41:A:HIS:HB3	5	0.19
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	1	0.19
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	4	0.19
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	14	0.19
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	12	0.18
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	15	0.18
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	11	0.18
(4,381)	1:140:A:THR:H	1:137:A:ARG:HB2	14	0.18
(4,379)	1:37:A:TYR:H	1:36:A:LYS:HG2	13	0.18
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	2	0.18
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	17	0.18
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	13	0.18
(4,346)	1:90:A:ASN:H	1:86:A:VAL:HA	18	0.18
(4,344)	1:39:A:TYR:H	1:96:A:LEU:HD21	6	0.18
(4,325)	1:133:A:ARG:H	1:133:A:ARG:HG2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,322)	1:86:A:VAL:H	1:82:A:ARG:HG2	8	0.18
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	19	0.18
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	4	0.18
(4,307)	1:110:A:PHE:H	1:78:A:LEU:HD11	17	0.18
(4,246)	1:13:A:THR:HA	1:93:A:LYS:HB3	9	0.18
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	7	0.18
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	13	0.18
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	7	0.18
(4,163)	1:166:A:ILE:HG21	1:170:A:GLU:HA	12	0.18
(4,155)	1:67:A:GLU:HA	1:67:A:GLU:HB3	10	0.18
(4,155)	1:8:A:GLU:HA	1:8:A:GLU:HG2	12	0.18
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	5	0.18
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	10	0.18
(4,94)	1:76:A:THR:HG21	1:75:A:GLU:HB2	11	0.18
(4,88)	1:76:A:THR:HG23	1:73:A:PRO:HB3	19	0.18
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	18	0.18
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	1	0.18
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	5	0.18
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	4	0.18
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	12	0.18
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	2	0.18
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	20	0.18
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	8	0.18
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	13	0.18
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	17	0.18
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	10	0.18
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	3	0.18
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	13	0.18
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	7	0.18
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	13	0.18
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	18	0.18
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	19	0.18
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	19	0.18
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	7	0.18
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	10	0.18
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	13	0.18
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	15	0.18
(1,2040)	1:108:A:GLU:H	1:106:A:GLN:HE21	11	0.18
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	2	0.18
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	7	0.18
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	4	0.18
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	1	0.18
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	4	0.18
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	7	0.18
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	8	0.18
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	16	0.18
(1,1907)	1:89:A:VAL:H	1:88:A:LYS:HZ1	16	0.18
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	1	0.18
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	16	0.18
(1,1882)	1:85:A:MET:H	1:86:A:VAL:HG11	10	0.18
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	16	0.18
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	1	0.18
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	4	0.18
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	5	0.18
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	7	0.18
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	19	0.18
(1,1790)	1:75:A:GLU:H	1:74:A:LEU:HD11	11	0.18
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	11	0.18
(1,1770)	1:70:A:GLN:H	1:70:A:GLN:HG3	1	0.18
(1,1638)	1:49:A:ARG:H	1:46:A:ASP:HB2	10	0.18
(1,1638)	1:49:A:ARG:H	1:46:A:ASP:HB2	11	0.18
(1,1578)	1:39:A:TYR:H	1:40:A:THR:H	12	0.18
(1,1537)	1:34:A:VAL:H	1:36:A:LYS:HA	17	0.18
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	4	0.18
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	8	0.18
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	9	0.18
(1,1363)	1:46:A:ASP:H	1:97:A:ILE:HG22	12	0.18
(1,1354)	1:182:A:GLY:H	1:187:A:VAL:HG23	4	0.18
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	12	0.18
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	5	0.18
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	10	0.18
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	12	0.18
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	9	0.18
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	18	0.18
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	3	0.18
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	10	0.18
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	8	0.18
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	15	0.18
(1,1110)	1:172:A:ARG:HA	1:172:A:ARG:HD3	17	0.18
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	8	0.18
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	11	0.18
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	14	0.18
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	9	0.18
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	20	0.18
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	6	0.18
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	1	0.18
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	15	0.18
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	18	0.18
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	8	0.18
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	5	0.18
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	7	0.18
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	5	0.18
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	6	0.18
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	1	0.18
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	1	0.18
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	6	0.18
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	9	0.18
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	14	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	2	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	9	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	10	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	11	0.18
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	14	0.18
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	14	0.18
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	17	0.18
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	17	0.18
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	7	0.18
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	11	0.18
(1,691)	1:92:A:SER:HB3	1:89:A:VAL:HG21	18	0.18
(1,681)	1:89:A:VAL:HG21	1:90:A:ASN:HA	1	0.18
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	17	0.18
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	8	0.18
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	12	0.18
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	17	0.18
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	3	0.18
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	18	0.18
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	17	0.18
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	5	0.18
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	10	0.18
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	17	0.18
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	8	0.18
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	14	0.18
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	2	0.18
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	8	0.18
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	14	0.18
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	16	0.18
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	16	0.18
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	13	0.18
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	10	0.18
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	13	0.18
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	2	0.18
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	7	0.18
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	9	0.18
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	7	0.18
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	9	0.18
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	13	0.18
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	14	0.18
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	3	0.18
(1,237)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	19	0.18
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	10	0.18
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	12	0.18
(1,226)	1:7:A:GLU:HA	1:6:A:MET:HA	20	0.18
(1,208)	1:152:A:LYS:HA	1:151:A:ILE:HG23	8	0.18
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	1	0.18
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	5	0.18
(1,106)	1:184:A:VAL:HG22	1:188:A:PHE:H	3	0.18
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	14	0.18
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	1	0.18
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	9	0.18
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	11	0.18
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	19	0.18
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	12	0.18
(1,1)	1:14:A:LYS:HG3	1:14:A:LYS:HA	15	0.18
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	10	0.17
(4,364)	1:150:A:THR:H	1:151:A:ILE:HA	13	0.17
(4,359)	1:169:A:TYR:H	1:171:A:LYS:HB2	1	0.17
(4,353)	1:85:A:MET:H	1:83:A:ASP:HB2	17	0.17
(4,349)	1:116:A:GLN:H	1:7:A:GLU:HG2	18	0.17
(4,345)	1:39:A:TYR:H	1:33:A:ILE:HG21	6	0.17
(4,339)	1:80:A:MET:H	1:47:A:LEU:HB3	13	0.17
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	17	0.17
(4,322)	1:86:A:VAL:H	1:87:A:ALA:HB2	18	0.17
(4,316)	1:130:A:MET:H	1:131:A:THR:HB	11	0.17
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	13	0.17
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	19	0.17
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	4	0.17
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	7	0.17
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	6	0.17
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	8	0.17
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	1	0.17
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	11	0.17
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	14	0.17
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	15	0.17
(4,146)	1:161:A:ALA:HB1	1:162:A:THR:HG1	19	0.17
(4,132)	1:184:A:VAL:HG22	1:188:A:PHE:HD2	14	0.17
(4,100)	1:19:A:VAL:HG13	1:169:A:TYR:HD1	17	0.17
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	9	0.17
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	20	0.17
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	19	0.17
(1,2561)	1:197:A:ALA:H	1:196:A:ASP:HB2	2	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	4	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	6	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	7	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	11	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	12	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	15	0.17
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	19	0.17
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	20	0.17
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	5	0.17
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	8	0.17
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	18	0.17
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	14	0.17
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	4	0.17
(1,2289)	1:156:A:GLU:H	1:152:A:LYS:HD3	13	0.17
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	4	0.17
(1,2274)	1:153:A:LYS:H	1:153:A:LYS:HG2	6	0.17
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	9	0.17
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	1	0.17
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	13	0.17
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	6	0.17
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	14	0.17
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	13	0.17
(1,2120)	1:122:A:TYR:H	1:122:A:TYR:HD1	8	0.17
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	15	0.17
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	1	0.17
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	18	0.17
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	14	0.17
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	14	0.17
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	5	0.17
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	7	0.17
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	9	0.17
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	1	0.17
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	7	0.17
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	18	0.17
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	2	0.17
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	9	0.17
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	3	0.17
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	13	0.17
(1,1770)	1:70:A:GLN:H	1:70:A:GLN:HG3	13	0.17
(1,1633)	1:48:A:LEU:H	1:47:A:LEU:HB2	6	0.17
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	9	0.17
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	4	0.17
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	7	0.17
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	8	0.17
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	13	0.17
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	17	0.17
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	13	0.17
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	6	0.17
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	17	0.17
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	9	0.17
(1,1301)	1:83:A:ASP:H	1:83:A:ASP:HB2	6	0.17
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	8	0.17
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	14	0.17
(1,1274)	1:61:A:LYS:H	1:61:A:LYS:HG3	15	0.17
(1,1274)	1:61:A:LYS:H	1:61:A:LYS:HG3	16	0.17
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	5	0.17
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	7	0.17
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	12	0.17
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	18	0.17
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	12	0.17
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	4	0.17
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	12	0.17
(1,1188)	1:185:A:ASP:HB2	1:183:A:SER:HB3	11	0.17
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	2	0.17
(1,1162)	1:178:A:VAL:HG11	1:190:A:GLN:HB2	18	0.17
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	3	0.17
(1,1107)	1:172:A:ARG:HA	1:171:A:LYS:HE3	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	11	0.17
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	8	0.17
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	5	0.17
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	9	0.17
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	2	0.17
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	17	0.17
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	15	0.17
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	3	0.17
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	19	0.17
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	8	0.17
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	12	0.17
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	13	0.17
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	17	0.17
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	3	0.17
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	5	0.17
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	11	0.17
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	14	0.17
(1,915)	1:137:A:ARG:HD3	1:135:A:LEU:HA	15	0.17
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	6	0.17
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	13	0.17
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	15	0.17
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	17	0.17
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	20	0.17
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	7	0.17
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	17	0.17
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	10	0.17
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	15	0.17
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	1	0.17
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	3	0.17
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	20	0.17
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	7	0.17
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	8	0.17
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	10	0.17
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	6	0.17
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	18	0.17
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	20	0.17
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	8	0.17
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	8	0.17
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	13	0.17
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	9	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	5	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	13	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	15	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	17	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	18	0.17
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	19	0.17
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	14	0.17
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	11	0.17
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	1	0.17
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	3	0.17
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	9	0.17
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	12	0.17
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	16	0.17
(1,613)	1:47:A:LEU:HG	1:84:A:ALA:HB1	2	0.17
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	2	0.17
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	8	0.17
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	12	0.17
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	15	0.17
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	16	0.17
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	18	0.17
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	19	0.17
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	2	0.17
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	8	0.17
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	1	0.17
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	14	0.17
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	15	0.17
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	1	0.17
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	18	0.17
(1,497)	1:57:A:ALA:HA	1:60:A:LYS:HE2	13	0.17
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	7	0.17
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	9	0.17
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	10	0.17
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	17	0.17
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	20	0.17
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	4	0.17
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	6	0.17
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	3	0.17
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	9	0.17
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	15	0.17
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	1	0.17
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	10	0.17
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	4	0.17
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	10	0.17
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	18	0.17
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	8	0.17
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	10	0.17
(1,230)	1:7:A:GLU:HB3	1:11:A:LYS:HE2	12	0.17
(1,208)	1:152:A:LYS:HA	1:151:A:ILE:HG23	3	0.17
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	8	0.17
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	2	0.17
(1,135)	1:114:A:ILE:HD11	1:82:A:ARG:HD3	3	0.17
(1,106)	1:184:A:VAL:HG22	1:188:A:PHE:H	18	0.17
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	4	0.17
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	19	0.17
(1,77)	1:34:A:VAL:HG11	1:41:A:HIS:HB3	9	0.17
(1,77)	1:34:A:VAL:HG11	1:41:A:HIS:HB3	13	0.17
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	15	0.17
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	17	0.17
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	7	0.17
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	19	0.16
(4,365)	1:56:A:SER:H	1:58:A:ARG:HB2	14	0.16
(4,346)	1:90:A:ASN:H	1:86:A:VAL:HA	12	0.16
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	5	0.16
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	7	0.16
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	8	0.16
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	2	0.16
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	4	0.16
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	10	0.16
(4,290)	1:100:A:TYR:H	1:19:A:VAL:HB	4	0.16
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	6	0.16
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	20	0.16
(4,243)	1:189:A:SER:HA	1:192:A:CYS:HB3	10	0.16
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	12	0.16
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	2	0.16
(4,163)	1:166:A:ILE:HG21	1:170:A:GLU:HA	5	0.16
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	18	0.16
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	7	0.16
(4,96)	1:76:A:THR:HG23	1:62:A:LEU:HD12	11	0.16
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	18	0.16
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	19	0.16
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	13	0.16
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	1	0.16
(4,16)	1:195:A:LEU:HD23	1:198:A:LEU:HB3	15	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	3	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	5	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	9	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	13	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	17	0.16
(1,2500)	1:187:A:VAL:H	1:187:A:VAL:HG21	20	0.16
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	6	0.16
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	7	0.16
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	19	0.16
(1,2426)	1:177:A:LYS:H	1:178:A:VAL:HG11	18	0.16
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	8	0.16
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	8	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	1	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	2	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	9	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	11	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	14	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	19	0.16
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	20	0.16
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	5	0.16
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	7	0.16
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	9	0.16
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	5	0.16
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	19	0.16
(1,2254)	1:149:A:GLU:H	1:153:A:LYS:HZ1	19	0.16
(1,2222)	1:144:A:VAL:H	1:143:A:ARG:HD3	14	0.16
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	3	0.16
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	20	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	1	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	5	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	10	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	15	0.16
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	20	0.16
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	1	0.16
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	2	0.16
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	15	0.16
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	5	0.16
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	3	0.16
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	8	0.16
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	11	0.16
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	17	0.16
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	3	0.16
(1,2090)	1:116:A:GLN:H	1:117:A:PRO:HD2	17	0.16
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	20	0.16
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	1	0.16
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	4	0.16
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	10	0.16
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	11	0.16
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	19	0.16
(1,2053)	1:111:A:GLU:H	1:111:A:GLU:HG2	1	0.16
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	1	0.16
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	9	0.16
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	6	0.16
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	7	0.16
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	9	0.16
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	20	0.16
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	12	0.16
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	17	0.16
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	19	0.16
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	1	0.16
(1,1944)	1:94:A:GLY:H	1:93:A:LYS:HE3	6	0.16
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	13	0.16
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	16	0.16
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	2	0.16
(1,1882)	1:85:A:MET:H	1:86:A:VAL:HG11	18	0.16
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	20	0.16
(1,1852)	1:82:A:ARG:H	1:83:A:ASP:HB2	19	0.16
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	5	0.16
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	14	0.16
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	17	0.16
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	7	0.16
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	18	0.16
(1,1690)	1:58:A:ARG:H	1:58:A:ARG:HE	15	0.16
(1,1690)	1:58:A:ARG:H	1:58:A:ARG:HE	20	0.16
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	9	0.16
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	19	0.16
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	12	0.16
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	13	0.16
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	14	0.16
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	16	0.16
(1,1530)	1:33:A:ILE:H	1:32:A:LYS:HB2	6	0.16
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	10	0.16
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	10	0.16
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	10	0.16
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	19	0.16
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	2	0.16
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	5	0.16
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	9	0.16
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	15	0.16
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	8	0.16
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	18	0.16
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	7	0.16
(1,1301)	1:83:A:ASP:H	1:83:A:ASP:HB2	5	0.16
(1,1300)	1:70:A:GLN:H	1:65:A:ILE:HG23	20	0.16
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	16	0.16
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	19	0.16
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	11	0.16
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	4	0.16
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	3	0.16
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	10	0.16
(1,1283)	1:146:A:ASP:H	1:151:A:ILE:HD13	1	0.16
(1,1242)	1:17:A:PHE:H	1:15:A:ILE:HD11	13	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	1	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	2	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	6	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	13	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	15	0.16
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	17	0.16
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	1	0.16
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	3	0.16
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	15	0.16
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	17	0.16
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	19	0.16
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	8	0.16
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	17	0.16
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	18	0.16
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	19	0.16
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	1	0.16
(1,1081)	1:166:A:ILE:HG21	1:122:A:TYR:HD2	4	0.16
(1,996)	1:152:A:LYS:HA	1:152:A:LYS:HD3	15	0.16
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	16	0.16
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	11	0.16
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	4	0.16
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	6	0.16
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	9	0.16
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	10	0.16
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	17	0.16
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	2	0.16
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	6	0.16
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	4	0.16
(1,895)	1:132:A:GLN:HB2	1:132:A:GLN:HG2	9	0.16
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	9	0.16
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	10	0.16
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	14	0.16
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	18	0.16
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	5	0.16
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	6	0.16
(1,822)	1:119:A:LEU:HD11	1:119:A:LEU:HB2	19	0.16
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	4	0.16
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	11	0.16
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	13	0.16
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	19	0.16
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	17	0.16
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	6	0.16
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	18	0.16
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	9	0.16
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	5	0.16
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	8	0.16
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	12	0.16
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	4	0.16
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	17	0.16
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	20	0.16
(1,705)	1:96:A:LEU:HG	1:195:A:LEU:HD21	10	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	1	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	6	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	8	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	16	0.16
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	20	0.16
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	6	0.16
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	17	0.16
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	3	0.16
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	6	0.16
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	17	0.16
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	1	0.16
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	15	0.16
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	6	0.16
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	8	0.16
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	6	0.16
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	19	0.16
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	5	0.16
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	9	0.16
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	16	0.16
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	9	0.16
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	8	0.16
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	11	0.16
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	3	0.16
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	12	0.16
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	7	0.16
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	15	0.16
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	8	0.16
(1,408)	1:36:A:LYS:HE3	1:36:A:LYS:HB3	16	0.16
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	9	0.16
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	2	0.16
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	7	0.16
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	8	0.16
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	17	0.16
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	1	0.16
(1,328)	1:19:A:VAL:HG21	1:121:A:LEU:HA	18	0.16
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	1	0.16
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	3	0.16
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	14	0.16
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	15	0.16
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	17	0.16
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	5	0.16
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	4	0.16
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	17	0.16
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	1	0.16
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	3	0.16
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	8	0.16
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	2	0.16
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	5	0.16
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	7	0.16
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	19	0.16
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	14	0.16
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	15	0.16
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:76:A:THR:HG23	1:58:A:ARG:HD2	7	0.16
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	3	0.16
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	7	0.16
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	3	0.16
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	13	0.16
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	16	0.16
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	12	0.16
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	19	0.16
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	19	0.15
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	7	0.15
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	1	0.15
(4,383)	1:23:A:GLY:H	1:26:A:LYS:HG3	6	0.15
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	4	0.15
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	8	0.15
(4,347)	1:90:A:ASN:H	1:9:A:LYS:HG2	16	0.15
(4,341)	1:80:A:MET:H	1:80:A:MET:HE3	19	0.15
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	10	0.15
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	14	0.15
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	19	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	1	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	5	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	6	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	7	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	9	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	11	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	13	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	14	0.15
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	15	0.15
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	6	0.15
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	9	0.15
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	10	0.15
(4,269)	1:7:A:GLU:HA	1:7:A:GLU:HB2	12	0.15
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	12	0.15
(4,243)	1:189:A:SER:HA	1:192:A:CYS:HB3	2	0.15
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	1	0.15
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	14	0.15
(4,222)	1:8:A:GLU:HA	1:8:A:GLU:HG2	15	0.15
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	9	0.15
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	3	0.15
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	8	0.15
(4,155)	1:8:A:GLU:HA	1:8:A:GLU:HG2	15	0.15
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	6	0.15
(4,96)	1:76:A:THR:HG22	1:62:A:LEU:HD12	13	0.15
(4,95)	1:76:A:THR:HG23	1:58:A:ARG:HG2	14	0.15
(4,72)	1:103:A:GLU:HA	1:164:A:PRO:HG2	20	0.15
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	2	0.15
(4,35)	1:61:A:LYS:HD2	1:62:A:LEU:HA	10	0.15
(4,17)	1:121:A:LEU:HG	1:194:A:HIS:HB2	8	0.15
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	6	0.15
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	19	0.15
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	9	0.15
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	10	0.15
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	17	0.15
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	7	0.15
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	10	0.15
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	20	0.15
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	3	0.15
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	6	0.15
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	7	0.15
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	10	0.15
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	6	0.15
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	13	0.15
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	20	0.15
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	1	0.15
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	17	0.15
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	6	0.15
(1,2197)	1:139:A:GLU:H	1:139:A:GLU:HG2	3	0.15
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	2	0.15
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	3	0.15
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	17	0.15
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	4	0.15
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	16	0.15
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	12	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	1	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	2	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	5	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	10	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	12	0.15
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	16	0.15
(1,2093)	1:119:A:LEU:H	1:15:A:ILE:HG21	11	0.15
(1,2063)	1:112:A:ARG:H	1:113:A:ARG:HG3	9	0.15
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	5	0.15
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2007)	1:104:A:VAL:H	1:105:A:GLN:H	15	0.15
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	4	0.15
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	12	0.15
(1,1993)	1:102:A:ARG:H	1:102:A:ARG:HD2	6	0.15
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	3	0.15
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	9	0.15
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	15	0.15
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	6	0.15
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	8	0.15
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	9	0.15
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	14	0.15
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	20	0.15
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	12	0.15
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	1	0.15
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	3	0.15
(1,1949)	1:95:A:PHE:H	1:15:A:ILE:HB	11	0.15
(1,1949)	1:95:A:PHE:H	1:15:A:ILE:HB	16	0.15
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	10	0.15
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	15	0.15
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	17	0.15
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	2	0.15
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	5	0.15
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	7	0.15
(1,1870)	1:84:A:ALA:H	1:85:A:MET:HB3	11	0.15
(1,1820)	1:79:A:ASP:H	1:77:A:VAL:HA	16	0.15
(1,1805)	1:76:A:THR:H	1:77:A:VAL:HG21	16	0.15
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	2	0.15
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	7	0.15
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	8	0.15
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	15	0.15
(1,1770)	1:70:A:GLN:H	1:70:A:GLN:HG3	9	0.15
(1,1652)	1:51:A:GLU:H	1:51:A:GLU:HG3	17	0.15
(1,1616)	1:45:A:GLY:H	1:43:A:SER:HB3	15	0.15
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	14	0.15
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	18	0.15
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	13	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	2	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	3	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	6	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	7	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	8	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	12	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	14	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	16	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	19	0.15
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	20	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	4	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	9	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	14	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	16	0.15
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	20	0.15
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	10	0.15
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	11	0.15
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	20	0.15
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	5	0.15
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	9	0.15
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	13	0.15
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	15	0.15
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	20	0.15
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	3	0.15
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	5	0.15
(1,1368)	1:63:A:SER:H	1:61:A:LYS:HG2	8	0.15
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	1	0.15
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	3	0.15
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	5	0.15
(1,1290)	1:10:A:LEU:H	1:10:A:LEU:HD11	13	0.15
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	13	0.15
(1,1279)	1:156:A:GLU:H	1:155:A:LEU:HD11	9	0.15
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	7	0.15
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	19	0.15
(1,1270)	1:155:A:LEU:H	1:152:A:LYS:HA	11	0.15
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	5	0.15
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	10	0.15
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	14	0.15
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	16	0.15
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	12	0.15
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	2	0.15
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	10	0.15
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	13	0.15
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	16	0.15
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	7	0.15
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	6	0.15
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	6	0.15
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	13	0.15
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	15	0.15
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	6	0.15
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	10	0.15
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	15	0.15
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	18	0.15
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	1	0.15
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	14	0.15
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	19	0.15
(1,1023)	1:159:A:TYR:HA	1:163:A:GLU:HG3	3	0.15
(1,1004)	1:156:A:GLU:HA	1:156:A:GLU:HG2	1	0.15
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	5	0.15
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	10	0.15
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	3	0.15
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	1	0.15
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	4	0.15
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	12	0.15
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	13	0.15
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	19	0.15
(1,903)	1:135:A:LEU:HD11	1:136:A:LYS:HA	9	0.15
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	13	0.15
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	15	0.15
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	19	0.15
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	14	0.15
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	16	0.15
(1,783)	1:113:A:ARG:HA	1:113:A:ARG:HD2	4	0.15
(1,776)	1:111:A:GLU:HG3	1:116:A:GLN:HA	4	0.15
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	17	0.15
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	13	0.15
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	3	0.15
(1,758)	1:104:A:VAL:HG21	1:104:A:VAL:HB	3	0.15
(1,758)	1:104:A:VAL:HG21	1:104:A:VAL:HB	15	0.15
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	4	0.15
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	13	0.15
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	17	0.15
(1,757)	1:104:A:VAL:HA	1:104:A:VAL:HG21	19	0.15
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	8	0.15
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	11	0.15
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	1	0.15
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	18	0.15
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	3	0.15
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	11	0.15
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	8	0.15
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	9	0.15
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	1	0.15
(1,587)	1:75:A:GLU:HA	1:74:A:LEU:HD11	7	0.15
(1,585)	1:74:A:LEU:HD11	1:106:A:GLN:HG2	19	0.15
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	2	0.15
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	17	0.15
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	18	0.15
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	10	0.15
(1,534)	1:64:A:GLU:HG2	1:68:A:LYS:HE3	15	0.15
(1,532)	1:63:A:SER:HA	1:62:A:LEU:HD11	7	0.15
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	2	0.15
(1,506)	1:58:A:ARG:HA	1:62:A:LEU:HD11	7	0.15
(1,497)	1:57:A:ALA:HA	1:60:A:LYS:HE2	2	0.15
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	4	0.15
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	19	0.15
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	15	0.15
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	5	0.15
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	15	0.15
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	3	0.15
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	5	0.15
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	7	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	2	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	3	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	7	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	9	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	11	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	12	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	14	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	15	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	16	0.15
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	20	0.15
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	5	0.15
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	6	0.15
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	20	0.15
(1,351)	1:26:A:LYS:HE2	1:26:A:LYS:HB2	17	0.15
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	10	0.15
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	13	0.15
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	13	0.15
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	19	0.15
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	16	0.15
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	6	0.15
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	13	0.15
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	20	0.15
(1,296)	1:16:A:ILE:HA	1:16:A:ILE:HG21	11	0.15
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	19	0.15
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	3	0.15
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	7	0.15
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	18	0.15
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	19	0.15
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	19	0.15
(1,207)	1:24:A:SER:HA	1:130:A:MET:HE1	9	0.15
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	4	0.15
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	7	0.15
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	17	0.15
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	20	0.15
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	10	0.15
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	20	0.15
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	2	0.15
(1,97)	1:52:A:VAL:HG11	1:58:A:ARG:HD2	6	0.15
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	9	0.15
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	3	0.15
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	8	0.15
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	5	0.15
(1,69)	1:191:A:VAL:HG12	1:187:A:VAL:HG22	13	0.15
(1,6)	1:12:A:LYS:HA	1:12:A:LYS:HD2	5	0.15
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	10	0.15
(4,397)	1:27:A:GLY:H	1:30:A:CYS:HB2	20	0.14
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	3	0.14
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	3	0.14
(4,357)	1:99:A:GLY:H	1:97:A:ILE:HB	1	0.14
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	2	0.14
(4,318)	1:65:A:ILE:H	1:62:A:LEU:HA	14	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	3	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	8	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	12	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	17	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	18	0.14
(4,311)	1:167:A:ALA:H	1:167:A:ALA:HA	20	0.14
(4,296)	1:46:A:ASP:H	1:48:A:LEU:HD21	5	0.14
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	18	0.14
(4,248)	1:63:A:SER:HA	1:49:A:ARG:HG2	15	0.14
(4,243)	1:189:A:SER:HA	1:192:A:CYS:HB3	12	0.14
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	5	0.14
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	12	0.14
(4,203)	1:7:A:GLU:HG2	1:7:A:GLU:HA	10	0.14
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	13	0.14
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	14	0.14
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	17	0.14
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	12	0.14
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	13	0.14
(4,155)	1:67:A:GLU:HG2	1:67:A:GLU:HA	1	0.14
(4,155)	1:105:A:GLN:HA	1:105:A:GLN:HG3	16	0.14
(4,141)	1:89:A:VAL:HG21	1:90:A:ASN:HB2	16	0.14
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	11	0.14
(4,97)	1:44:A:THR:HG22	1:100:A:TYR:HA	17	0.14
(4,66)	1:78:A:LEU:HD21	1:74:A:LEU:HB2	3	0.14
(4,50)	1:88:A:LYS:HG3	1:88:A:LYS:HE2	1	0.14
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	10	0.14
(1,2578)	1:199:A:LYS:H	1:199:A:LYS:HE2	16	0.14
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	8	0.14
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	15	0.14
(1,2448)	1:180:A:ALA:H	1:124:A:ASP:HB2	15	0.14
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	12	0.14
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	3	0.14
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	13	0.14
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	15	0.14
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	8	0.14
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	10	0.14
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	7	0.14
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	18	0.14
(1,2283)	1:155:A:LEU:H	1:154:A:ARG:HH11	18	0.14
(1,2247)	1:148:A:GLU:H	1:147:A:ASN:HB3	17	0.14
(1,2238)	1:146:A:ASP:H	1:147:A:ASN:HD22	15	0.14
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	19	0.14
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	9	0.14
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	17	0.14
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	11	0.14
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	12	0.14
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	18	0.14
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	19	0.14
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2040)	1:108:A:GLU:H	1:106:A:GLN:HE21	9	0.14
(1,2040)	1:108:A:GLU:H	1:106:A:GLN:HE21	17	0.14
(1,2025)	1:106:A:GLN:H	1:106:A:GLN:HE21	9	0.14
(1,2007)	1:104:A:VAL:H	1:105:A:GLN:H	3	0.14
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	1	0.14
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	5	0.14
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	8	0.14
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	10	0.14
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	16	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	5	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	6	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	12	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	14	0.14
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	18	0.14
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	2	0.14
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	13	0.14
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	16	0.14
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	20	0.14
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	11	0.14
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	17	0.14
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	12	0.14
(1,1779)	1:72:A:VAL:H	1:72:A:VAL:HG11	2	0.14
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	4	0.14
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	5	0.14
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	18	0.14
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	9	0.14
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	15	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	1	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	4	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	5	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	6	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	7	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	8	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	10	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	12	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	13	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	17	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	18	0.14
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	19	0.14
(1,1689)	1:58:A:ARG:H	1:58:A:ARG:HD2	7	0.14
(1,1664)	1:53:A:SER:H	1:53:A:SER:HB2	13	0.14
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	13	0.14
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	20	0.14
(1,1633)	1:48:A:LEU:H	1:47:A:LEU:HB2	8	0.14
(1,1615)	1:45:A:GLY:H	1:43:A:SER:HB2	3	0.14
(1,1517)	1:31:A:GLU:H	1:30:A:CYS:HB2	8	0.14
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	17	0.14
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	14	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	1	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	4	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	5	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	9	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	15	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	17	0.14
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	18	0.14
(1,1435)	1:16:A:ILE:H	1:97:A:ILE:HB	17	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	1	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	2	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	5	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	7	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	8	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	11	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	12	0.14
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	13	0.14
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	3	0.14
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	18	0.14
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	4	0.14
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	7	0.14
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	13	0.14
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	8	0.14
(1,1296)	1:129:A:THR:H	1:128:A:GLU:HG3	19	0.14
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	20	0.14
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	6	0.14
(1,1256)	1:100:A:TYR:H	1:97:A:ILE:HG23	1	0.14
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	7	0.14
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	9	0.14
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	11	0.14
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	20	0.14
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	5	0.14
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	9	0.14
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	15	0.14
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	19	0.14
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	1	0.14
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	16	0.14
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	3	0.14
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	11	0.14
(1,1112)	1:172:A:ARG:HD3	1:171:A:LYS:HB3	19	0.14
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	4	0.14
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	12	0.14
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	17	0.14
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	2	0.14
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	9	0.14
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	18	0.14
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	15	0.14
(1,969)	1:151:A:ILE:HA	1:154:A:ARG:HD2	16	0.14
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	5	0.14
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	6	0.14
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	16	0.14
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	7	0.14
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	8	0.14
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	18	0.14
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	20	0.14
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	5	0.14
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	7	0.14
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	10	0.14
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	20	0.14
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	12	0.14
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	17	0.14
(1,908)	1:135:A:LEU:HD11	1:148:A:GLU:HA	14	0.14
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	2	0.14
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	4	0.14
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	12	0.14
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	2	0.14
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	8	0.14
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	18	0.14
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	1	0.14
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	12	0.14
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	19	0.14
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	18	0.14
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	2	0.14
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	4	0.14
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	5	0.14
(1,789)	1:114:A:ILE:HD11	1:79:A:ASP:HA	20	0.14
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	19	0.14
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	11	0.14
(1,759)	1:104:A:VAL:HG11	1:104:A:VAL:HG21	16	0.14
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	10	0.14
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	19	0.14
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	12	0.14
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	12	0.14
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	5	0.14
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	20	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	3	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	4	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	6	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	7	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	8	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	9	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	10	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	11	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	12	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	13	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	14	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	15	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	17	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	18	0.14
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	19	0.14
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	4	0.14
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	5	0.14
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	13	0.14
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	15	0.14
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	16	0.14
(1,655)	1:87:A:ALA:HB1	1:88:A:LYS:HB2	18	0.14
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	10	0.14
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	19	0.14
(1,587)	1:75:A:GLU:HA	1:74:A:LEU:HD11	2	0.14
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	3	0.14
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	7	0.14
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	10	0.14
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	20	0.14
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	11	0.14
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	13	0.14
(1,515)	1:59:A:GLY:HA3	1:63:A:SER:HB3	14	0.14
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	9	0.14
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	14	0.14
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	19	0.14
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	13	0.14
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	9	0.14
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	14	0.14
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	17	0.14
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	13	0.14
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	2	0.14
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	10	0.14
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	14	0.14
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	15	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	1	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	4	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	6	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	8	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	10	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	13	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	17	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	18	0.14
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	19	0.14
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	7	0.14
(1,393)	1:34:A:VAL:HG21	1:35:A:GLN:HE21	5	0.14
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	15	0.14
(1,347)	1:26:A:LYS:HB2	1:26:A:LYS:HE3	7	0.14
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	12	0.14
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	20	0.14
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	9	0.14
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	3	0.14
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	17	0.14
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	6	0.14
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	9	0.14
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	10	0.14
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	15	0.14
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	17	0.14
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	3	0.14
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	8	0.14
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	16	0.14
(1,220)	1:80:A:MET:HA	1:83:A:ASP:HB2	20	0.14
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	11	0.14
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	13	0.14
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	17	0.14
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	20	0.14
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	13	0.14
(1,134)	1:96:A:LEU:HG	1:34:A:VAL:HG13	12	0.14
(1,121)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	17	0.14
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	7	0.14
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	17	0.14
(1,42)	1:113:A:ARG:HG3	1:78:A:LEU:HA	17	0.14
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	16	0.14
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	18	0.14
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	2	0.14
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	14	0.14
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	6	0.13
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	8	0.13
(4,341)	1:80:A:MET:H	1:48:A:LEU:HD22	2	0.13
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	1	0.13
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	8	0.13
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	8	0.13
(4,292)	1:159:A:TYR:H	1:156:A:GLU:HG3	16	0.13
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	1	0.13
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	4	0.13
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	13	0.13
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	20	0.13
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	16	0.13
(4,145)	1:104:A:VAL:HG21	1:161:A:ALA:HA	16	0.13
(4,92)	1:76:A:THR:HG21	1:80:A:MET:HG3	4	0.13
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	8	0.13
(4,41)	1:35:A:GLN:HA	1:35:A:GLN:HG2	7	0.13
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	8	0.13
(4,16)	1:195:A:LEU:HD23	1:198:A:LEU:HB3	6	0.13
(1,2475)	1:182:A:GLY:H	1:183:A:SER:HG	18	0.13
(1,2426)	1:177:A:LYS:H	1:178:A:VAL:HG11	14	0.13
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	18	0.13
(1,2404)	1:174:A:ILE:H	1:175:A:VAL:HG11	8	0.13
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	4	0.13
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	15	0.13
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	11	0.13
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	9	0.13
(1,2272)	1:153:A:LYS:H	1:152:A:LYS:HE3	13	0.13
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	5	0.13
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	12	0.13
(1,2216)	1:143:A:ARG:H	1:143:A:ARG:HD2	11	0.13
(1,2150)	1:126:A:GLY:H	1:125:A:ALA:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	1:124:A:ASP:H	1:180:A:ALA:HB1	16	0.13
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	20	0.13
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	8	0.13
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	19	0.13
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	4	0.13
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	6	0.13
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	7	0.13
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	14	0.13
(1,2082)	1:116:A:GLN:H	1:15:A:ILE:HG21	11	0.13
(1,2081)	1:114:A:ILE:H	1:114:A:ILE:HG13	17	0.13
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	7	0.13
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	8	0.13
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	3	0.13
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	19	0.13
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	10	0.13
(1,2009)	1:105:A:GLN:H	1:103:A:GLU:HG2	3	0.13
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	1	0.13
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	20	0.13
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	8	0.13
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	10	0.13
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	20	0.13
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	15	0.13
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	19	0.13
(1,1965)	1:97:A:ILE:H	1:95:A:PHE:HB2	15	0.13
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	2	0.13
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	16	0.13
(1,1958)	1:96:A:LEU:H	1:95:A:PHE:HB2	7	0.13
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	12	0.13
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	8	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	8	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	9	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	11	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	12	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	15	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	16	0.13
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	19	0.13
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	1	0.13
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	6	0.13
(1,1720)	1:63:A:SER:H	1:62:A:LEU:HB3	5	0.13
(1,1717)	1:63:A:SER:H	1:59:A:GLY:HA2	3	0.13
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	5	0.13
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	8	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	2	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	3	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	9	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	11	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	14	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	16	0.13
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	20	0.13
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	6	0.13
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	2	0.13
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	14	0.13
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	18	0.13
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	1	0.13
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	4	0.13
(1,1601)	1:42:A:LEU:H	1:96:A:LEU:HB2	15	0.13
(1,1543)	1:36:A:LYS:H	1:33:A:ILE:H	9	0.13
(1,1543)	1:36:A:LYS:H	1:33:A:ILE:H	16	0.13
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	12	0.13
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	14	0.13
(1,1517)	1:31:A:GLU:H	1:30:A:CYS:HB2	11	0.13
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	6	0.13
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	4	0.13
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	10	0.13
(1,1469)	1:19:A:VAL:H	1:20:A:GLY:H	13	0.13
(1,1438)	1:16:A:ILE:H	1:17:A:PHE:H	13	0.13
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	4	0.13
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	3	0.13
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	6	0.13
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	17	0.13
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	18	0.13
(1,1401)	1:12:A:LYS:H	1:11:A:LYS:HA	12	0.13
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	3	0.13
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	14	0.13
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	13	0.13
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	14	0.13
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	12	0.13
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	1	0.13
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	3	0.13
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	4	0.13
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	7	0.13
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	19	0.13
(1,1297)	1:132:A:GLN:H	1:130:A:MET:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	2	0.13
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	4	0.13
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	7	0.13
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	20	0.13
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	3	0.13
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	8	0.13
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	8	0.13
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	14	0.13
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	16	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	2	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	3	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	12	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	13	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	17	0.13
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	18	0.13
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	13	0.13
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	1	0.13
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	6	0.13
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	7	0.13
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	20	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	1	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	2	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	5	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	10	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	11	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	13	0.13
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	20	0.13
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	2	0.13
(1,1118)	1:172:A:ARG:HD2	1:174:A:ILE:HG21	11	0.13
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	3	0.13
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	11	0.13
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	17	0.13
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	19	0.13
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	18	0.13
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	3	0.13
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	5	0.13
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	7	0.13
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	12	0.13
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	12	0.13
(1,1059)	1:165:A:VAL:HG11	1:106:A:GLN:HE21	16	0.13
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	18	0.13
(1,977)	1:151:A:ILE:HD11	1:135:A:LEU:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	14	0.13
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	18	0.13
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	7	0.13
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	9	0.13
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	12	0.13
(1,939)	1:144:A:VAL:HA	1:144:A:VAL:HG21	14	0.13
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	1	0.13
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	9	0.13
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	1	0.13
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	7	0.13
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	12	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	1	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	2	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	5	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	6	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	7	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	8	0.13
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	14	0.13
(1,889)	1:131:A:THR:HG21	1:135:A:LEU:HD11	14	0.13
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	11	0.13
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	8	0.13
(1,814)	1:118:A:THR:HG21	1:118:A:THR:HA	13	0.13
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	18	0.13
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	1	0.13
(1,789)	1:114:A:ILE:HD11	1:79:A:ASP:HA	12	0.13
(1,770)	1:110:A:PHE:HA	1:114:A:ILE:HG13	20	0.13
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	2	0.13
(1,765)	1:103:A:GLU:HA	1:106:A:GLN:HB2	17	0.13
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	7	0.13
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	9	0.13
(1,739)	1:102:A:ARG:HA	1:102:A:ARG:HD2	12	0.13
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	7	0.13
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	9	0.13
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	20	0.13
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	10	0.13
(1,723)	1:97:A:ILE:HG12	1:42:A:LEU:HD21	15	0.13
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	1	0.13
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	2	0.13
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	16	0.13
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	1	0.13
(1,675)	1:89:A:VAL:HG11	1:95:A:PHE:HE2	10	0.13
(1,672)	1:89:A:VAL:HG11	1:88:A:LYS:HE2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	14	0.13
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	13	0.13
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	18	0.13
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	20	0.13
(1,638)	1:84:A:ALA:HA	1:83:A:ASP:HB3	1	0.13
(1,638)	1:84:A:ALA:HA	1:83:A:ASP:HB3	5	0.13
(1,638)	1:84:A:ALA:HA	1:83:A:ASP:HB3	6	0.13
(1,638)	1:84:A:ALA:HA	1:83:A:ASP:HB3	20	0.13
(1,588)	1:75:A:GLU:HA	1:113:A:ARG:HD2	16	0.13
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	1	0.13
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	5	0.13
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	9	0.13
(1,562)	1:71:A:LEU:HA	1:71:A:LEU:HB2	13	0.13
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	14	0.13
(1,552)	1:65:A:ILE:HA	1:68:A:LYS:HD2	17	0.13
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	7	0.13
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	3	0.13
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	3	0.13
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	6	0.13
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	8	0.13
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	10	0.13
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	1	0.13
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	4	0.13
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	10	0.13
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	6	0.13
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	8	0.13
(1,462)	1:44:A:THR:HG21	1:48:A:LEU:HG	7	0.13
(1,462)	1:44:A:THR:HG21	1:48:A:LEU:HG	19	0.13
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	14	0.13
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	18	0.13
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	19	0.13
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	4	0.13
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	8	0.13
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	17	0.13
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	4	0.13
(1,399)	1:35:A:GLN:HA	1:34:A:VAL:HA	5	0.13
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	17	0.13
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	4	0.13
(1,351)	1:26:A:LYS:HE2	1:26:A:LYS:HB2	15	0.13
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	10	0.13
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	12	0.13
(1,329)	1:19:A:VAL:HG21	1:122:A:TYR:HD1	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	20	0.13
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	4	0.13
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	18	0.13
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	7	0.13
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	12	0.13
(1,296)	1:16:A:ILE:HA	1:16:A:ILE:HG21	20	0.13
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	12	0.13
(1,273)	1:15:A:ILE:HD11	1:15:A:ILE:HG13	20	0.13
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	10	0.13
(1,262)	1:14:A:LYS:HA	1:14:A:LYS:HB3	6	0.13
(1,259)	1:13:A:THR:HG21	1:14:A:LYS:HB2	12	0.13
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	5	0.13
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	17	0.13
(1,253)	1:11:A:LYS:HB2	1:12:A:LYS:HA	20	0.13
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	12	0.13
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	9	0.13
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	18	0.13
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	8	0.13
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	15	0.13
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	19	0.13
(1,153)	1:166:A:ILE:HD12	1:162:A:THR:HG1	1	0.13
(1,153)	1:166:A:ILE:HD12	1:162:A:THR:HG1	19	0.13
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	1	0.13
(1,108)	1:34:A:VAL:HG23	1:40:A:THR:HA	17	0.13
(1,89)	1:191:A:VAL:HG22	1:195:A:LEU:HD22	10	0.13
(1,81)	1:76:A:THR:HG21	1:58:A:ARG:HD2	15	0.13
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	6	0.13
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	4	0.13
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	8	0.13
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	11	0.13
(4,370)	1:50:A:SER:H	1:80:A:MET:HE1	19	0.12
(4,323)	1:10:A:LEU:H	1:89:A:VAL:HG12	20	0.12
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	2	0.12
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	9	0.12
(4,289)	1:158:A:TYR:H	1:162:A:THR:HB	16	0.12
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	12	0.12
(4,286)	1:51:A:GLU:H	1:58:A:ARG:HD3	14	0.12
(4,280)	1:179:A:ASN:H	1:187:A:VAL:HG21	3	0.12
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	1	0.12
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	13	0.12
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	18	0.12
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	16	0.12
(4,222)	1:51:A:GLU:HA	1:51:A:GLU:HG2	18	0.12
(4,210)	1:170:A:GLU:HG2	1:170:A:GLU:HA	4	0.12
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	10	0.12
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	16	0.12
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HG2	2	0.12
(4,187)	1:58:A:ARG:HA	1:58:A:ARG:HG2	3	0.12
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	5	0.12
(4,116)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	4	0.12
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	1	0.12
(4,41)	1:35:A:GLN:HA	1:35:A:GLN:HG2	5	0.12
(4,20)	1:74:A:LEU:HG	1:106:A:GLN:HB3	19	0.12
(4,9)	1:134:A:LEU:HG	1:134:A:LEU:HB3	15	0.12
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	1	0.12
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	17	0.12
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	5	0.12
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	7	0.12
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	8	0.12
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	15	0.12
(1,2505)	1:188:A:PHE:H	1:187:A:VAL:HA	14	0.12
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	4	0.12
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	2	0.12
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	3	0.12
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	17	0.12
(1,2424)	1:177:A:LYS:H	1:177:A:LYS:HE2	18	0.12
(1,2420)	1:177:A:LYS:H	1:176:A:ARG:HG2	14	0.12
(1,2417)	1:176:A:ARG:H	1:177:A:LYS:HG3	11	0.12
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	15	0.12
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	17	0.12
(1,2384)	1:172:A:ARG:H	1:169:A:TYR:HA	16	0.12
(1,2379)	1:170:A:GLU:H	1:172:A:ARG:H	17	0.12
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	3	0.12
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	18	0.12
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	6	0.12
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	18	0.12
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	19	0.12
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	19	0.12
(1,2300)	1:158:A:TYR:H	1:156:A:GLU:H	3	0.12
(1,2300)	1:158:A:TYR:H	1:156:A:GLU:H	10	0.12
(1,2280)	1:154:A:ARG:H	1:154:A:ARG:HD2	9	0.12
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	7	0.12
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	15	0.12
(1,2255)	1:150:A:THR:H	1:135:A:LEU:HD21	19	0.12
(1,2253)	1:149:A:GLU:H	1:148:A:GLU:HG3	16	0.12
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	20	0.12
(1,2161)	1:129:A:THR:H	1:128:A:GLU:HG2	12	0.12
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	7	0.12
(1,2124)	1:123:A:VAL:H	1:18:A:VAL:HG21	4	0.12
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	3	0.12
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	6	0.12
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	16	0.12
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	9	0.12
(1,2082)	1:116:A:GLN:H	1:15:A:ILE:HG21	5	0.12
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	11	0.12
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	13	0.12
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	18	0.12
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	1	0.12
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	20	0.12
(1,2039)	1:108:A:GLU:H	1:104:A:VAL:HG21	11	0.12
(1,2023)	1:106:A:GLN:H	1:104:A:VAL:HA	3	0.12
(1,2007)	1:104:A:VAL:H	1:105:A:GLN:H	17	0.12
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	13	0.12
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	18	0.12
(1,2001)	1:103:A:GLU:H	1:106:A:GLN:HG2	19	0.12
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	13	0.12
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	5	0.12
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	19	0.12
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	2	0.12
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	11	0.12
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	13	0.12
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	19	0.12
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	2	0.12
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	5	0.12
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	6	0.12
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	14	0.12
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	11	0.12
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	1	0.12
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	7	0.12
(1,1900)	1:88:A:LYS:H	1:89:A:VAL:HB	8	0.12
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	4	0.12
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	8	0.12
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	9	0.12
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	2	0.12
(1,1853)	1:82:A:ARG:H	1:113:A:ARG:HD2	6	0.12
(1,1820)	1:79:A:ASP:H	1:77:A:VAL:HA	19	0.12
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	1	0.12
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	6	0.12
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	14	0.12
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	20	0.12
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	16	0.12
(1,1770)	1:70:A:GLN:H	1:70:A:GLN:HG3	4	0.12
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	1	0.12
(1,1694)	1:59:A:GLY:H	1:58:A:ARG:HA	15	0.12
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	6	0.12
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	11	0.12
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	14	0.12
(1,1601)	1:42:A:LEU:H	1:96:A:LEU:HB2	17	0.12
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	2	0.12
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	16	0.12
(1,1517)	1:31:A:GLU:H	1:30:A:CYS:HB2	4	0.12
(1,1517)	1:31:A:GLU:H	1:30:A:CYS:HB2	18	0.12
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	14	0.12
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	1	0.12
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	6	0.12
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	7	0.12
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	11	0.12
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	19	0.12
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	12	0.12
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	2	0.12
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	9	0.12
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	14	0.12
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	16	0.12
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	20	0.12
(1,1411)	1:13:A:THR:H	1:14:A:LYS:H	15	0.12
(1,1401)	1:12:A:LYS:H	1:11:A:LYS:HA	2	0.12
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	7	0.12
(1,1391)	1:9:A:LYS:H	1:89:A:VAL:HG11	14	0.12
(1,1390)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	0.12
(1,1384)	1:9:A:LYS:H	1:6:A:MET:HA	20	0.12
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	19	0.12
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	7	0.12
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	18	0.12
(1,1339)	1:88:A:LYS:H	1:40:A:THR:HG21	13	0.12
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	14	0.12
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG12	18	0.12
(1,1320)	1:12:A:LYS:H	1:12:A:LYS:HD2	20	0.12
(1,1310)	1:116:A:GLN:H	1:114:A:ILE:HG21	7	0.12
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	16	0.12
(1,1287)	1:82:A:ARG:H	1:85:A:MET:HG3	1	0.12
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	11	0.12
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	15	0.12
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	4	0.12
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	9	0.12
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	11	0.12
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	20	0.12
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	4	0.12
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	8	0.12
(1,1228)	1:197:A:ALA:HA	1:198:A:LEU:HD11	2	0.12
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	6	0.12
(1,1205)	1:191:A:VAL:HG21	1:29:A:GLN:HG2	2	0.12
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	4	0.12
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	17	0.12
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	19	0.12
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	20	0.12
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	6	0.12
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	17	0.12
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	18	0.12
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	1	0.12
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	9	0.12
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	15	0.12
(1,1100)	1:168:A:PHE:HA	1:172:A:ARG:H	13	0.12
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	4	0.12
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	15	0.12
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	18	0.12
(1,1082)	1:166:A:ILE:HG21	1:163:A:GLU:HB2	16	0.12
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	6	0.12
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	8	0.12
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	11	0.12
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	13	0.12
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	4	0.12
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	7	0.12
(1,980)	1:151:A:ILE:HD11	1:148:A:GLU:HB2	14	0.12
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	11	0.12
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	15	0.12
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	12	0.12
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	17	0.12
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	18	0.12
(1,928)	1:141:A:SER:HB3	1:141:A:SER:HA	4	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	4	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	9	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	10	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	13	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	15	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	16	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	18	0.12
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	19	0.12
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	2	0.12
(1,876)	1:131:A:THR:HG21	1:128:A:GLU:HA	20	0.12
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	4	0.12
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	1	0.12
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	5	0.12
(1,830)	1:121:A:LEU:HA	1:176:A:ARG:HG2	8	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	1	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	3	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	7	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	10	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	12	0.12
(1,816)	1:118:A:THR:HG21	1:119:A:LEU:H	17	0.12
(1,814)	1:118:A:THR:HG21	1:118:A:THR:HA	15	0.12
(1,802)	1:113:A:ARG:HG3	1:114:A:ILE:HG21	20	0.12
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	2	0.12
(1,800)	1:114:A:ILE:HG21	1:81:A:LEU:H	6	0.12
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	13	0.12
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	17	0.12
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	13	0.12
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	20	0.12
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	9	0.12
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	11	0.12
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	17	0.12
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	2	0.12
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	2	0.12
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	13	0.12
(1,737)	1:101:A:PRO:HA	1:101:A:PRO:HD2	16	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	3	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	4	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	8	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	14	0.12
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	19	0.12
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	2	0.12
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	3	0.12
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	7	0.12
(1,719)	1:97:A:ILE:HD11	1:97:A:ILE:HG21	17	0.12
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	2	0.12
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	13	0.12
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	16	0.12
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	19	0.12
(1,682)	1:90:A:ASN:HA	1:90:A:ASN:HB2	20	0.12
(1,670)	1:6:A:MET:HA	1:89:A:VAL:HG11	12	0.12
(1,605)	1:78:A:LEU:HA	1:113:A:ARG:HD2	4	0.12
(1,549)	1:68:A:LYS:HA	1:68:A:LYS:HE2	6	0.12
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	7	0.12
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	11	0.12
(1,539)	1:65:A:ILE:HB	1:70:A:GLN:HB3	15	0.12
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	18	0.12
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	5	0.12
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	19	0.12
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	18	0.12
(1,439)	1:42:A:LEU:HA	1:47:A:LEU:HG	10	0.12
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	17	0.12
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	18	0.12
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	1	0.12
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	14	0.12
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	20	0.12
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	10	0.12
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	19	0.12
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	10	0.12
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	11	0.12
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	19	0.12
(1,337)	1:23:A:GLY:HA2	1:133:A:ARG:HD3	10	0.12
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	5	0.12
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	14	0.12
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	3	0.12
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	19	0.12
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	13	0.12
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	15	0.12
(1,257)	1:13:A:THR:HG21	1:10:A:LEU:HA	12	0.12
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	7	0.12
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	8	0.12
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	12	0.12
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	14	0.12
(1,251)	1:10:A:LEU:HD21	1:115:A:GLY:HA2	13	0.12
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	6	0.12
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	13	0.12
(1,208)	1:152:A:LYS:HA	1:151:A:ILE:HG23	4	0.12
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	1	0.12
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	6	0.12
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	9	0.12
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	12	0.12
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	16	0.12
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	4	0.12
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	5	0.12
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	9	0.12
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	10	0.12
(1,154)	1:76:A:THR:HB	1:48:A:LEU:HA	20	0.12
(1,149)	1:13:A:THR:HB	1:89:A:VAL:HG12	15	0.12
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	10	0.12
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	15	0.12
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	12	0.12
(1,95)	1:184:A:VAL:HG11	1:25:A:GLY:HA2	9	0.12
(1,91)	1:134:A:LEU:HD12	1:135:A:LEU:HA	3	0.12
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	6	0.12
(1,25)	1:74:A:LEU:HG	1:73:A:PRO:HA	15	0.12
(4,391)	1:38:A:GLY:H	1:33:A:ILE:HG21	14	0.11
(4,383)	1:45:A:GLY:H	1:48:A:LEU:HB2	5	0.11
(4,379)	1:37:A:TYR:H	1:36:A:LYS:HG2	11	0.11
(4,364)	1:150:A:THR:H	1:151:A:ILE:HA	14	0.11
(4,359)	1:169:A:TYR:H	1:171:A:LYS:HB2	11	0.11
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	7	0.11
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	16	0.11
(4,328)	1:153:A:LYS:H	1:150:A:THR:HA	18	0.11
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	1	0.11
(4,305)	1:155:A:LEU:H	1:156:A:GLU:HG2	20	0.11
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	3	0.11
(4,218)	1:65:A:ILE:HA	1:70:A:GLN:HB3	3	0.11
(4,217)	1:47:A:LEU:HD12	1:43:A:SER:HB3	12	0.11
(4,209)	1:8:A:GLU:HA	1:8:A:GLU:HG2	15	0.11
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	4	0.11
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,202)	1:149:A:GLU:HG2	1:150:A:THR:HA	12	0.11
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	4	0.11
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	7	0.11
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	10	0.11
(4,170)	1:151:A:ILE:HD13	1:135:A:LEU:HB3	17	0.11
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	3	0.11
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	4	0.11
(4,155)	1:105:A:GLN:HA	1:105:A:GLN:HG3	4	0.11
(4,146)	1:161:A:ALA:HB1	1:162:A:THR:HG1	1	0.11
(4,146)	1:161:A:ALA:HB2	1:157:A:THR:HA	7	0.11
(4,116)	1:134:A:LEU:HD11	1:22:A:PRO:HG3	8	0.11
(4,114)	1:162:A:THR:HG21	1:165:A:VAL:HB	17	0.11
(4,97)	1:44:A:THR:HG21	1:44:A:THR:HA	7	0.11
(4,95)	1:76:A:THR:HG23	1:58:A:ARG:HG2	10	0.11
(4,88)	1:34:A:VAL:HG12	1:31:A:GLU:HB3	4	0.11
(4,41)	1:132:A:GLN:HA	1:132:A:GLN:HG2	4	0.11
(4,41)	1:35:A:GLN:HA	1:35:A:GLN:HG2	16	0.11
(4,16)	1:195:A:LEU:HD23	1:198:A:LEU:HB3	19	0.11
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	13	0.11
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	18	0.11
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	1	0.11
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	4	0.11
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	9	0.11
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	10	0.11
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	12	0.11
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	1	0.11
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	6	0.11
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	18	0.11
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	4	0.11
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	16	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	5	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	8	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	10	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	14	0.11
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	20	0.11
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	2	0.11
(1,2328)	1:162:A:THR:H	1:162:A:THR:HG21	12	0.11
(1,2321)	1:161:A:ALA:H	1:160:A:LYS:HE3	11	0.11
(1,2267)	1:152:A:LYS:H	1:151:A:ILE:HD11	13	0.11
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	13	0.11
(1,2220)	1:144:A:VAL:H	1:143:A:ARG:HB2	19	0.11
(1,2170)	1:133:A:ARG:H	1:133:A:ARG:HD2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	9	0.11
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	7	0.11
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	10	0.11
(1,2122)	1:122:A:TYR:H	1:178:A:VAL:H	13	0.11
(1,2120)	1:122:A:TYR:H	1:122:A:TYR:HD1	11	0.11
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	19	0.11
(1,2098)	1:119:A:LEU:H	1:120:A:LEU:HB3	20	0.11
(1,2093)	1:119:A:LEU:H	1:15:A:ILE:HG21	16	0.11
(1,2082)	1:116:A:GLN:H	1:15:A:ILE:HG21	12	0.11
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	15	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	9	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	10	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	12	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	14	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	17	0.11
(1,2059)	1:112:A:ARG:H	1:111:A:GLU:HG2	20	0.11
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	7	0.11
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	8	0.11
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	14	0.11
(1,2007)	1:104:A:VAL:H	1:105:A:GLN:H	11	0.11
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	8	0.11
(1,1995)	1:102:A:ARG:H	1:106:A:GLN:HB2	11	0.11
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	3	0.11
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	4	0.11
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	6	0.11
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	11	0.11
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	4	0.11
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	7	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	4	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	7	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	8	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	9	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	10	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	17	0.11
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	20	0.11
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	17	0.11
(1,1949)	1:95:A:PHE:H	1:15:A:ILE:HB	18	0.11
(1,1949)	1:95:A:PHE:H	1:15:A:ILE:HB	20	0.11
(1,1935)	1:92:A:SER:H	1:95:A:PHE:HZ	12	0.11
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	3	0.11
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	14	0.11
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1854)	1:82:A:ARG:H	1:113:A:ARG:HE	7	0.11
(1,1826)	1:79:A:ASP:H	1:113:A:ARG:HH11	5	0.11
(1,1820)	1:79:A:ASP:H	1:77:A:VAL:HA	20	0.11
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	2	0.11
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	13	0.11
(1,1775)	1:72:A:VAL:H	1:71:A:LEU:H	17	0.11
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	19	0.11
(1,1772)	1:71:A:LEU:H	1:70:A:GLN:HB2	20	0.11
(1,1748)	1:67:A:GLU:H	1:67:A:GLU:HG2	13	0.11
(1,1720)	1:63:A:SER:H	1:62:A:LEU:HB3	8	0.11
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	17	0.11
(1,1707)	1:61:A:LYS:H	1:61:A:LYS:HZ1	19	0.11
(1,1658)	1:53:A:SER:H	1:49:A:ARG:HD3	5	0.11
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	1	0.11
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	7	0.11
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	9	0.11
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	12	0.11
(1,1656)	1:52:A:VAL:H	1:59:A:GLY:HA3	17	0.11
(1,1652)	1:51:A:GLU:H	1:51:A:GLU:HG3	15	0.11
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	15	0.11
(1,1605)	1:43:A:SER:H	1:42:A:LEU:HG	13	0.11
(1,1601)	1:42:A:LEU:H	1:96:A:LEU:HB2	19	0.11
(1,1570)	1:39:A:TYR:H	1:37:A:TYR:HD1	13	0.11
(1,1570)	1:39:A:TYR:H	1:37:A:TYR:HD1	18	0.11
(1,1553)	1:37:A:TYR:H	1:35:A:GLN:HB2	20	0.11
(1,1529)	1:33:A:ILE:H	1:31:A:GLU:HA	7	0.11
(1,1515)	1:30:A:CYS:H	1:31:A:GLU:HG3	10	0.11
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	2	0.11
(1,1513)	1:30:A:CYS:H	1:29:A:GLN:HG3	18	0.11
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	12	0.11
(1,1507)	1:30:A:CYS:H	1:26:A:LYS:HB3	13	0.11
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	9	0.11
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	15	0.11
(1,1435)	1:16:A:ILE:H	1:97:A:ILE:HB	20	0.11
(1,1423)	1:15:A:ILE:H	1:14:A:LYS:HG3	12	0.11
(1,1418)	1:14:A:LYS:H	1:15:A:ILE:HA	12	0.11
(1,1383)	1:8:A:GLU:H	1:7:A:GLU:HB3	9	0.11
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	4	0.11
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	6	0.11
(1,1375)	1:6:A:MET:H	1:6:A:MET:HG2	7	0.11
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	9	0.11
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:182:A:GLY:H	1:187:A:VAL:HG11	18	0.11
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	6	0.11
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	11	0.11
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	15	0.11
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	17	0.11
(1,1332)	1:189:A:SER:H	1:29:A:GLN:HE22	20	0.11
(1,1321)	1:11:A:LYS:H	1:89:A:VAL:HG11	17	0.11
(1,1301)	1:83:A:ASP:H	1:83:A:ASP:HB2	20	0.11
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	9	0.11
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	14	0.11
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	4	0.11
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	16	0.11
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	17	0.11
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	20	0.11
(1,1274)	1:61:A:LYS:H	1:61:A:LYS:HG3	11	0.11
(1,1274)	1:61:A:LYS:H	1:61:A:LYS:HG3	19	0.11
(1,1235)	1:198:A:LEU:HA	1:198:A:LEU:HD11	1	0.11
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	16	0.11
(1,1198)	1:187:A:VAL:HG21	1:191:A:VAL:HB	18	0.11
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	6	0.11
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	7	0.11
(1,1191)	1:187:A:VAL:HG11	1:183:A:SER:HA	18	0.11
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	3	0.11
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	9	0.11
(1,1180)	1:184:A:VAL:HG11	1:29:A:GLN:HG3	16	0.11
(1,1179)	1:181:A:GLU:HA	1:181:A:GLU:HG2	17	0.11
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	3	0.11
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	12	0.11
(1,1178)	1:181:A:GLU:HB2	1:181:A:GLU:HA	16	0.11
(1,1100)	1:168:A:PHE:HA	1:172:A:ARG:H	1	0.11
(1,1100)	1:168:A:PHE:HA	1:172:A:ARG:H	19	0.11
(1,1090)	1:166:A:ILE:HG21	1:175:A:VAL:HG11	8	0.11
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	2	0.11
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	7	0.11
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	14	0.11
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	16	0.11
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	5	0.11
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	8	0.11
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	13	0.11
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	16	0.11
(1,1061)	1:165:A:VAL:HG11	1:162:A:THR:HA	20	0.11
(1,1028)	1:161:A:ALA:HA	1:160:A:LYS:HE3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:154:A:ARG:HA	1:154:A:ARG:HD2	8	0.11
(1,994)	1:152:A:LYS:HA	1:151:A:ILE:HG21	9	0.11
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	8	0.11
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	15	0.11
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	1	0.11
(1,959)	1:149:A:GLU:HG3	1:152:A:LYS:HE3	4	0.11
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	10	0.11
(1,957)	1:149:A:GLU:HG2	1:149:A:GLU:HA	14	0.11
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	11	0.11
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	13	0.11
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	15	0.11
(1,931)	1:143:A:ARG:HA	1:143:A:ARG:HD2	1	0.11
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	2	0.11
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	4	0.11
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	5	0.11
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	10	0.11
(1,928)	1:141:A:SER:HB3	1:141:A:SER:HA	19	0.11
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	3	0.11
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	11	0.11
(1,921)	1:139:A:GLU:HA	1:139:A:GLU:HB3	20	0.11
(1,900)	1:133:A:ARG:HD2	1:134:A:LEU:HB3	11	0.11
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	9	0.11
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	11	0.11
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	17	0.11
(1,883)	1:134:A:LEU:HD11	1:131:A:THR:HA	3	0.11
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	7	0.11
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	2	0.11
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	13	0.11
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	14	0.11
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	7	0.11
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	10	0.11
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	1	0.11
(1,836)	1:121:A:LEU:HD11	1:16:A:ILE:HG21	2	0.11
(1,799)	1:114:A:ILE:HG21	1:15:A:ILE:HG13	18	0.11
(1,795)	1:113:A:ARG:HG3	1:114:A:ILE:HD11	8	0.11
(1,795)	1:113:A:ARG:HG3	1:114:A:ILE:HD11	10	0.11
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	19	0.11
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	6	0.11
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	7	0.11
(1,789)	1:114:A:ILE:HD11	1:79:A:ASP:HA	8	0.11
(1,763)	1:106:A:GLN:HA	1:105:A:GLN:HG2	20	0.11
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	14	0.11
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	18	0.11
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	19	0.11
(1,747)	1:103:A:GLU:HG2	1:102:A:ARG:HD3	17	0.11
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	6	0.11
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	12	0.11
(1,722)	1:97:A:ILE:HD11	1:110:A:PHE:HE2	4	0.11
(1,719)	1:97:A:ILE:HD11	1:97:A:ILE:HG21	5	0.11
(1,719)	1:97:A:ILE:HD11	1:97:A:ILE:HG21	6	0.11
(1,708)	1:96:A:LEU:HG	1:41:A:HIS:HD2	1	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	1	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	3	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	6	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	7	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	8	0.11
(1,698)	1:95:A:PHE:HA	1:95:A:PHE:HE1	14	0.11
(1,696)	1:95:A:PHE:HA	1:42:A:LEU:HD21	12	0.11
(1,671)	1:89:A:VAL:HG11	1:86:A:VAL:HA	17	0.11
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	8	0.11
(1,627)	1:81:A:LEU:HD11	1:84:A:ALA:HB1	12	0.11
(1,610)	1:78:A:LEU:HD11	1:110:A:PHE:HD1	11	0.11
(1,608)	1:78:A:LEU:HD11	1:74:A:LEU:HD21	15	0.11
(1,584)	1:74:A:LEU:HD11	1:106:A:GLN:HE22	15	0.11
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	11	0.11
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	14	0.11
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	9	0.11
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	9	0.11
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	4	0.11
(1,509)	1:58:A:ARG:HD2	1:58:A:ARG:HA	16	0.11
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	1	0.11
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	9	0.11
(1,454)	1:43:A:SER:HB3	1:46:A:ASP:HB2	15	0.11
(1,442)	1:43:A:SER:HA	1:41:A:HIS:HD2	1	0.11
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	2	0.11
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	7	0.11
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	11	0.11
(1,424)	1:40:A:THR:HG21	1:41:A:HIS:HA	16	0.11
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	13	0.11
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	18	0.11
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	19	0.11
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	11	0.11
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:35:A:GLN:HA	1:32:A:LYS:HA	15	0.11
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	2	0.11
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	6	0.11
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	7	0.11
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	12	0.11
(1,383)	1:33:A:ILE:HG21	1:39:A:TYR:HD1	15	0.11
(1,380)	1:33:A:ILE:HG21	1:37:A:TYR:HE1	15	0.11
(1,348)	1:26:A:LYS:HB2	1:123:A:VAL:HG21	10	0.11
(1,334)	1:134:A:LEU:HD11	1:22:A:PRO:HB3	14	0.11
(1,330)	1:22:A:PRO:HA	1:23:A:GLY:HA3	6	0.11
(1,314)	1:18:A:VAL:HG11	1:26:A:LYS:HA	5	0.11
(1,306)	1:17:A:PHE:HA	1:15:A:ILE:HD11	18	0.11
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	1	0.11
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	6	0.11
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	13	0.11
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	14	0.11
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	7	0.11
(1,288)	1:18:A:VAL:HG11	1:16:A:ILE:HD11	13	0.11
(1,273)	1:15:A:ILE:HD11	1:15:A:ILE:HG13	13	0.11
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	8	0.11
(1,263)	1:14:A:LYS:HA	1:14:A:LYS:HE2	12	0.11
(1,252)	1:10:A:LEU:HD21	1:115:A:GLY:HA3	9	0.11
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	15	0.11
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	5	0.11
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	10	0.11
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	3	0.11
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	6	0.11
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	11	0.11
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	16	0.11
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	19	0.11
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	17	0.11
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	18	0.11
(1,143)	1:134:A:LEU:HB3	1:130:A:MET:HA	19	0.11
(1,121)	1:114:A:ILE:HG21	1:115:A:GLY:HA2	18	0.11
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	3	0.11
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	4	0.11
(1,35)	1:143:A:ARG:HG2	1:143:A:ARG:HD2	4	0.11
(1,4)	1:57:A:ALA:HA	1:60:A:LYS:HD3	4	0.11
(4,371)	1:50:A:SER:H	1:46:A:ASP:HB2	12	0.1
(4,364)	1:150:A:THR:H	1:151:A:ILE:HA	4	0.1
(4,364)	1:150:A:THR:H	1:151:A:ILE:HA	20	0.1
(4,350)	1:116:A:GLN:H	1:15:A:ILE:HB	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	6	0.1
(4,312)	1:167:A:ALA:H	1:166:A:ILE:HG22	16	0.1
(4,276)	1:104:A:VAL:H	1:106:A:GLN:HE21	17	0.1
(4,254)	1:58:A:ARG:HA	1:58:A:ARG:HB2	7	0.1
(4,224)	1:103:A:GLU:HB2	1:161:A:ALA:HA	18	0.1
(4,223)	1:49:A:ARG:HA	1:66:A:MET:HG2	5	0.1
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	10	0.1
(4,176)	1:172:A:ARG:HD2	1:117:A:PRO:HB2	12	0.1
(4,163)	1:174:A:ILE:HG21	1:173:A:GLY:HA2	19	0.1
(4,162)	1:16:A:ILE:HG23	1:121:A:LEU:HG	3	0.1
(4,155)	1:105:A:GLN:HA	1:105:A:GLN:HG3	6	0.1
(4,155)	1:105:A:GLN:HA	1:105:A:GLN:HG3	19	0.1
(4,8)	1:134:A:LEU:HG	1:134:A:LEU:HB2	1	0.1
(1,2569)	1:198:A:LEU:H	1:197:A:ALA:HB1	3	0.1
(1,2520)	1:190:A:GLN:H	1:192:A:CYS:H	11	0.1
(1,2488)	1:185:A:ASP:H	1:185:A:ASP:HB2	17	0.1
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	2	0.1
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	3	0.1
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	8	0.1
(1,2469)	1:182:A:GLY:H	1:180:A:ALA:HB1	14	0.1
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	9	0.1
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	14	0.1
(1,2430)	1:178:A:VAL:H	1:124:A:ASP:HA	16	0.1
(1,2416)	1:176:A:ARG:H	1:177:A:LYS:HE2	3	0.1
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	9	0.1
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	11	0.1
(1,2410)	1:176:A:ARG:H	1:119:A:LEU:HD21	14	0.1
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	11	0.1
(1,2339)	1:162:A:THR:HG21	1:165:A:VAL:H	17	0.1
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	4	0.1
(1,2335)	1:165:A:VAL:H	1:104:A:VAL:HA	13	0.1
(1,2289)	1:156:A:GLU:H	1:152:A:LYS:HD3	9	0.1
(1,2289)	1:156:A:GLU:H	1:152:A:LYS:HD3	19	0.1
(1,2273)	1:153:A:LYS:H	1:153:A:LYS:HE3	3	0.1
(1,2226)	1:145:A:ASP:H	1:143:A:ARG:HA	14	0.1
(1,2197)	1:139:A:GLU:H	1:139:A:GLU:HG2	7	0.1
(1,2186)	1:137:A:ARG:H	1:137:A:ARG:HB2	10	0.1
(1,2126)	1:123:A:VAL:H	1:26:A:LYS:HG2	3	0.1
(1,2120)	1:122:A:TYR:H	1:122:A:TYR:HD1	4	0.1
(1,2093)	1:119:A:LEU:H	1:15:A:ILE:HG21	13	0.1
(1,2093)	1:119:A:LEU:H	1:15:A:ILE:HG21	18	0.1
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2075)	1:114:A:ILE:H	1:110:A:PHE:HD2	6	0.1
(1,2055)	1:111:A:GLU:H	1:169:A:TYR:HE2	9	0.1
(1,2023)	1:106:A:GLN:H	1:104:A:VAL:HA	15	0.1
(1,2021)	1:106:A:GLN:H	1:103:A:GLU:HG3	9	0.1
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	7	0.1
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	9	0.1
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	10	0.1
(1,1989)	1:102:A:ARG:H	1:100:A:TYR:HD2	16	0.1
(1,1972)	1:98:A:ASP:H	1:97:A:ILE:HG21	16	0.1
(1,1968)	1:97:A:ILE:H	1:98:A:ASP:H	12	0.1
(1,1964)	1:97:A:ILE:H	1:17:A:PHE:HD1	15	0.1
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	2	0.1
(1,1956)	1:95:A:PHE:H	1:95:A:PHE:HE1	15	0.1
(1,1925)	1:91:A:THR:H	1:92:A:SER:HB3	2	0.1
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	6	0.1
(1,1885)	1:86:A:VAL:H	1:82:A:ARG:HA	7	0.1
(1,1882)	1:85:A:MET:H	1:86:A:VAL:HG11	13	0.1
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	14	0.1
(1,1863)	1:84:A:ALA:H	1:80:A:MET:HB2	17	0.1
(1,1720)	1:63:A:SER:H	1:62:A:LEU:HB3	12	0.1
(1,1684)	1:58:A:ARG:H	1:56:A:SER:HA	13	0.1
(1,1638)	1:49:A:ARG:H	1:46:A:ASP:HB2	7	0.1
(1,1635)	1:48:A:LEU:H	1:48:A:LEU:HD11	6	0.1
(1,1633)	1:48:A:LEU:H	1:47:A:LEU:HB2	17	0.1
(1,1632)	1:48:A:LEU:H	1:44:A:THR:HB	20	0.1
(1,1619)	1:45:A:GLY:H	1:46:A:ASP:HB2	7	0.1
(1,1605)	1:43:A:SER:H	1:42:A:LEU:HG	18	0.1
(1,1570)	1:39:A:TYR:H	1:37:A:TYR:HD1	5	0.1
(1,1553)	1:37:A:TYR:H	1:35:A:GLN:HB2	14	0.1
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	12	0.1
(1,1504)	1:29:A:GLN:H	1:29:A:GLN:HG2	13	0.1
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	12	0.1
(1,1503)	1:29:A:GLN:H	1:29:A:GLN:HE21	20	0.1
(1,1473)	1:20:A:GLY:H	1:26:A:LYS:HD2	2	0.1
(1,1435)	1:16:A:ILE:H	1:97:A:ILE:HB	4	0.1
(1,1435)	1:16:A:ILE:H	1:97:A:ILE:HB	6	0.1
(1,1422)	1:15:A:ILE:H	1:14:A:LYS:HG2	11	0.1
(1,1414)	1:14:A:LYS:H	1:14:A:LYS:HB2	15	0.1
(1,1401)	1:12:A:LYS:H	1:11:A:LYS:HA	17	0.1
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	11	0.1
(1,1366)	1:60:A:LYS:H	1:52:A:VAL:HA	20	0.1
(1,1292)	1:118:A:THR:H	1:14:A:LYS:HA	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	9	0.1
(1,1289)	1:186:A:SER:H	1:185:A:ASP:HB2	14	0.1
(1,1276)	1:28:A:THR:H	1:26:A:LYS:HA	9	0.1
(1,1241)	1:19:A:VAL:H	1:120:A:LEU:HA	19	0.1
(1,1206)	1:191:A:VAL:HG21	1:191:A:VAL:HA	18	0.1
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	5	0.1
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	11	0.1
(1,1194)	1:180:A:ALA:HA	1:187:A:VAL:HG21	13	0.1
(1,1190)	1:180:A:ALA:HB1	1:187:A:VAL:HG11	16	0.1
(1,1161)	1:178:A:VAL:HG11	1:187:A:VAL:HB	14	0.1
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	1	0.1
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	6	0.1
(1,1088)	1:166:A:ILE:HG21	1:167:A:ALA:HB1	10	0.1
(1,1080)	1:166:A:ILE:HG13	1:177:A:LYS:HE3	15	0.1
(1,1079)	1:166:A:ILE:HG13	1:162:A:THR:HA	19	0.1
(1,989)	1:151:A:ILE:HG21	1:148:A:GLU:HA	15	0.1
(1,961)	1:149:A:GLU:HG3	1:153:A:LYS:HB3	7	0.1
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	3	0.1
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	4	0.1
(1,936)	1:144:A:VAL:HB	1:145:A:ASP:HA	17	0.1
(1,930)	1:143:A:ARG:HA	1:143:A:ARG:HB2	6	0.1
(1,928)	1:141:A:SER:HB3	1:141:A:SER:HA	16	0.1
(1,899)	1:133:A:ARG:HB2	1:133:A:ARG:HG3	4	0.1
(1,888)	1:131:A:THR:HG21	1:132:A:GLN:HG2	1	0.1
(1,888)	1:131:A:THR:HG21	1:132:A:GLN:HG2	14	0.1
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	10	0.1
(1,878)	1:129:A:THR:HB	1:128:A:GLU:HG3	15	0.1
(1,870)	1:125:A:ALA:HB1	1:130:A:MET:HG2	10	0.1
(1,864)	1:124:A:ASP:HB3	1:177:A:LYS:HD2	8	0.1
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	4	0.1
(1,842)	1:195:A:LEU:HD21	1:121:A:LEU:HD11	14	0.1
(1,795)	1:113:A:ARG:HG3	1:114:A:ILE:HD11	12	0.1
(1,793)	1:114:A:ILE:HD11	1:110:A:PHE:HD2	1	0.1
(1,792)	1:82:A:ARG:HA	1:114:A:ILE:HD11	3	0.1
(1,751)	1:104:A:VAL:HA	1:104:A:VAL:HG11	6	0.1
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	2	0.1
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	15	0.1
(1,736)	1:101:A:PRO:HA	1:100:A:TYR:HD2	17	0.1
(1,719)	1:97:A:ILE:HD11	1:97:A:ILE:HG21	14	0.1
(1,679)	1:89:A:VAL:HA	1:89:A:VAL:HG21	7	0.1
(1,644)	1:85:A:MET:HA	1:86:A:VAL:HG21	6	0.1
(1,619)	1:81:A:LEU:HB3	1:78:A:LEU:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:78:A:LEU:HD11	1:110:A:PHE:HD1	13	0.1
(1,598)	1:77:A:VAL:HG11	1:100:A:TYR:HE1	1	0.1
(1,577)	1:73:A:PRO:HD3	1:72:A:VAL:HG21	10	0.1
(1,567)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	4	0.1
(1,560)	1:70:A:GLN:HG3	1:71:A:LEU:HD11	13	0.1
(1,531)	1:62:A:LEU:HD11	1:66:A:MET:HE1	4	0.1
(1,530)	1:62:A:LEU:HD11	1:62:A:LEU:HD21	20	0.1
(1,481)	1:49:A:ARG:HA	1:48:A:LEU:HB2	11	0.1
(1,470)	1:46:A:ASP:HB2	1:49:A:ARG:HB2	15	0.1
(1,462)	1:44:A:THR:HG21	1:48:A:LEU:HG	2	0.1
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	1	0.1
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	9	0.1
(1,429)	1:40:A:THR:HG21	1:92:A:SER:HA	19	0.1
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	4	0.1
(1,405)	1:35:A:GLN:HA	1:35:A:GLN:HG2	10	0.1
(1,387)	1:34:A:VAL:HA	1:96:A:LEU:HD21	18	0.1
(1,385)	1:195:A:LEU:HD21	1:33:A:ILE:HG21	7	0.1
(1,385)	1:195:A:LEU:HD21	1:33:A:ILE:HG21	14	0.1
(1,385)	1:195:A:LEU:HD21	1:33:A:ILE:HG21	17	0.1
(1,383)	1:33:A:ILE:HG21	1:39:A:TYR:HD1	3	0.1
(1,380)	1:33:A:ILE:HG21	1:37:A:TYR:HE1	3	0.1
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	1	0.1
(1,374)	1:33:A:ILE:HA	1:35:A:GLN:HG2	5	0.1
(1,331)	1:22:A:PRO:HA	1:26:A:LYS:HB2	1	0.1
(1,300)	1:16:A:ILE:HG21	1:119:A:LEU:H	16	0.1
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	9	0.1
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	10	0.1
(1,299)	1:16:A:ILE:HG21	1:18:A:VAL:HG11	20	0.1
(1,277)	1:15:A:ILE:HD11	1:110:A:PHE:HZ	18	0.1
(1,273)	1:15:A:ILE:HD11	1:15:A:ILE:HG13	19	0.1
(1,269)	1:14:A:LYS:HD3	1:15:A:ILE:HA	15	0.1
(1,255)	1:13:A:THR:HB	1:89:A:VAL:HG11	13	0.1
(1,240)	1:10:A:LEU:HA	1:12:A:LYS:HG2	11	0.1
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	2	0.1
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	3	0.1
(1,191)	1:178:A:VAL:HG13	1:123:A:VAL:HA	13	0.1
(1,179)	1:40:A:THR:HA	1:38:A:GLY:HA2	7	0.1
(1,154)	1:76:A:THR:HB	1:48:A:LEU:HA	9	0.1
(1,154)	1:76:A:THR:HB	1:48:A:LEU:HA	14	0.1
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	8	0.1
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	9	0.1
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:40:A:THR:HB	1:95:A:PHE:HD2	18	0.1
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	8	0.1
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	11	0.1
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	18	0.1
(1,110)	1:127:A:PRO:HD3	1:128:A:GLU:HA	20	0.1
(1,16)	1:133:A:ARG:HG3	1:132:A:GLN:HB2	11	0.1

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

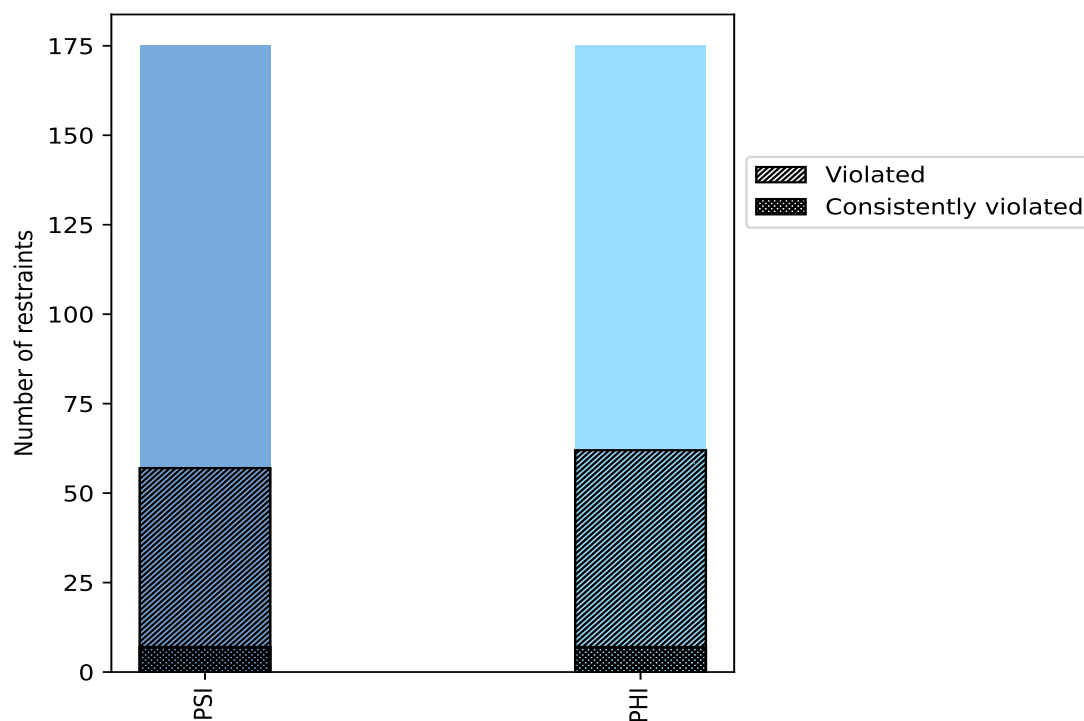
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	175	50.0	57	32.6	16.3	7	4.0	2.0
PHI	175	50.0	62	35.4	17.7	7	4.0	2.0
Total	350	100.0	119	34.0	34.0	14	4.0	4.0

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](#)



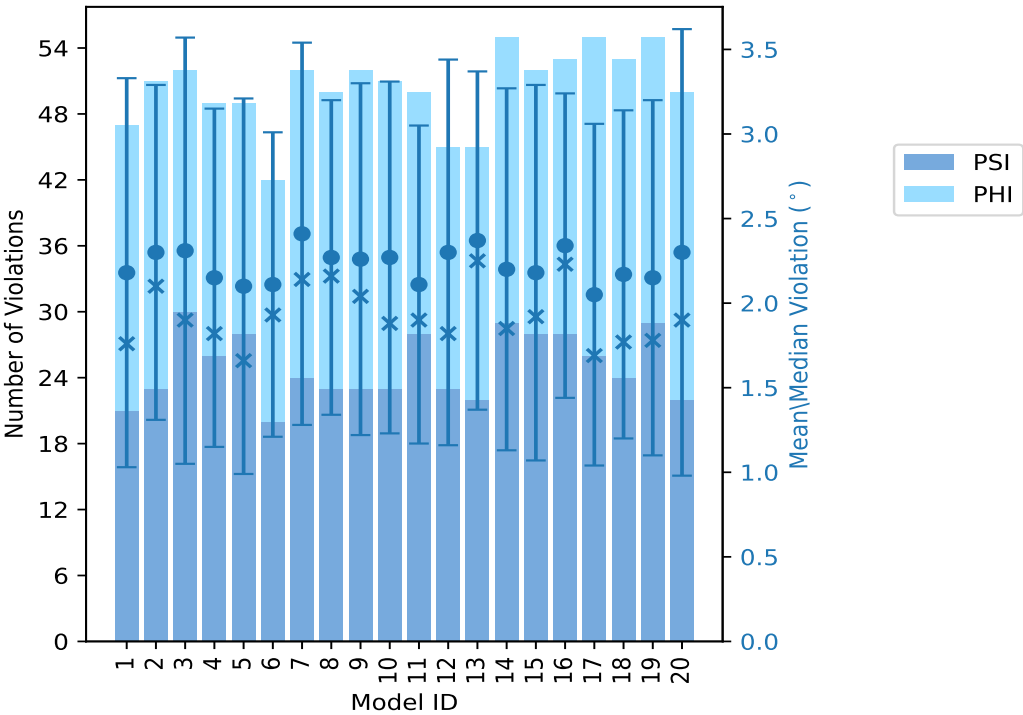
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	21	26	47	2.18	6.35	1.15	1.76
2	23	28	51	2.3	5.61	0.99	2.1
3	30	22	52	2.31	5.66	1.26	1.9
4	26	23	49	2.15	4.73	1.0	1.82
5	28	21	49	2.1	5.46	1.11	1.66
6	20	22	42	2.11	4.7	0.9	1.93
7	24	28	52	2.41	5.63	1.13	2.14
8	23	27	50	2.27	5.19	0.93	2.16
9	23	29	52	2.26	5.14	1.04	2.04
10	23	28	51	2.27	5.52	1.04	1.88
11	28	22	50	2.11	4.89	0.94	1.9
12	23	22	45	2.3	5.36	1.14	1.82
13	22	23	45	2.37	5.64	1.0	2.25
14	29	26	55	2.2	5.38	1.07	1.85
15	28	24	52	2.18	6.62	1.11	1.92
16	28	25	53	2.34	5.05	0.9	2.23
17	26	29	55	2.05	5.3	1.01	1.69
18	24	29	53	2.17	5.3	0.97	1.77
19	29	26	55	2.15	5.03	1.05	1.78
20	22	28	50	2.3	6.49	1.32	1.9

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	
PSI	PHI	Total	Count ¹	%
9	7	16	1	5.0
5	9	14	2	10.0
7	5	12	3	15.0
0	6	6	4	20.0
4	3	7	5	25.0
2	1	3	6	30.0
4	4	8	7	35.0
2	4	6	8	40.0
0	2	2	9	45.0
1	3	4	10	50.0
1	2	3	11	55.0

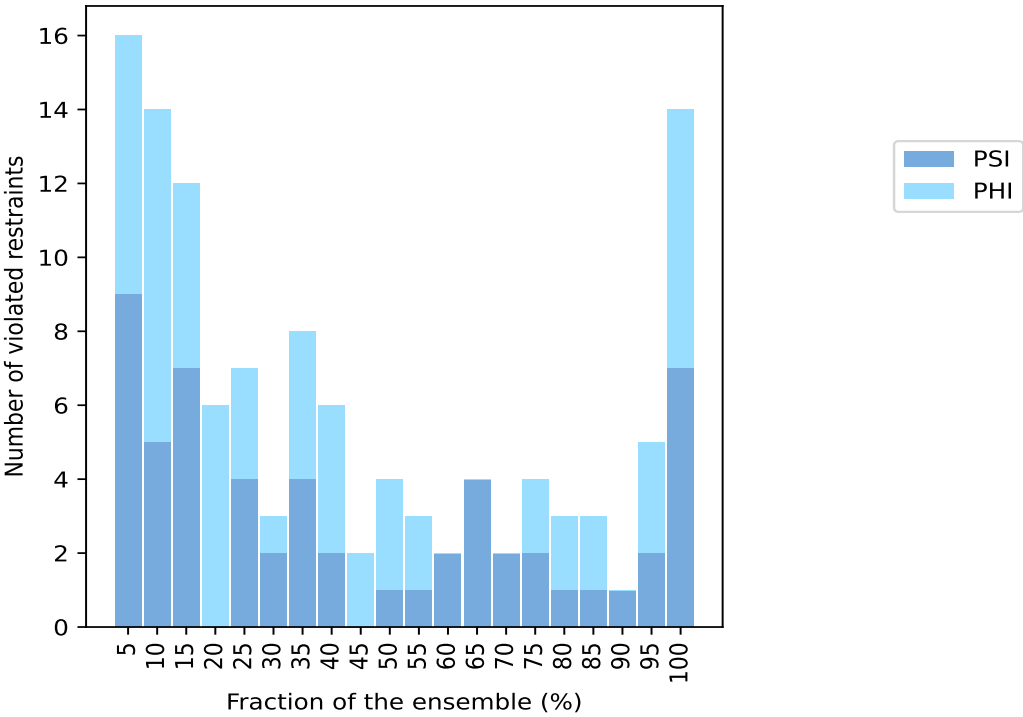
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
2	0	2	12	60.0
4	0	4	13	65.0
2	0	2	14	70.0
2	2	4	15	75.0
1	2	3	16	80.0
1	2	3	17	85.0
1	0	1	18	90.0
2	3	5	19	95.0
7	7	14	20	100.0

¹ Number of models with violations

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

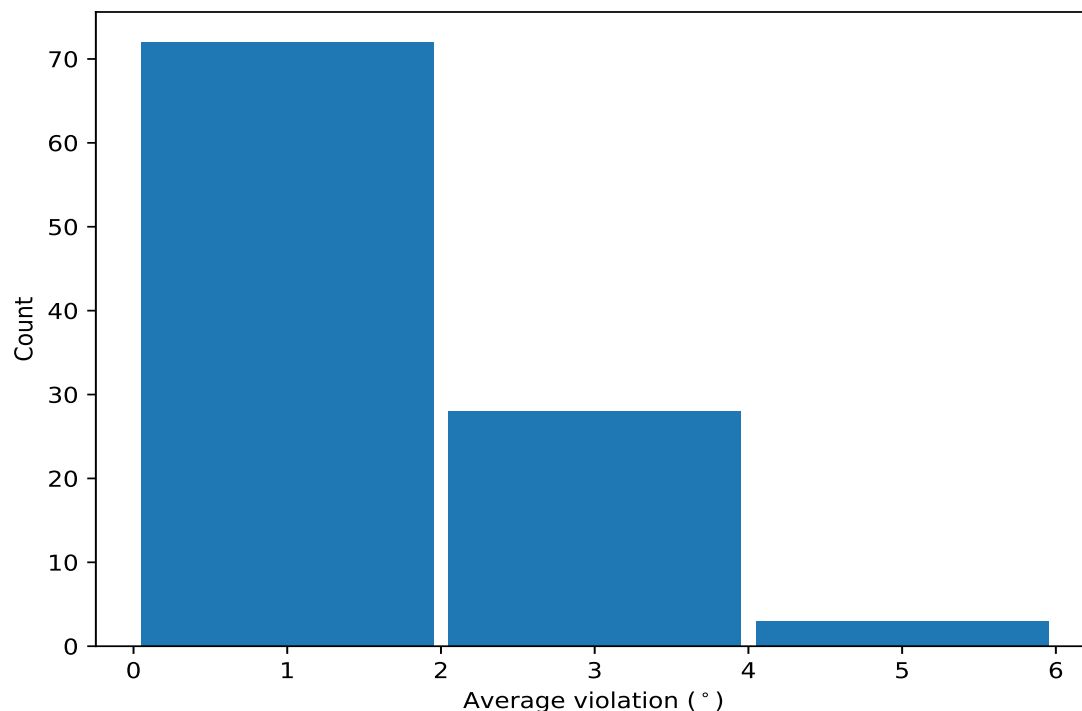


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	20	4.71	0.73	4.7
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	20	4.29	1.37	4.75
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	20	4.02	0.73	4.11
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	20	3.74	1.08	3.52
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	20	3.42	0.61	3.39
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	20	3.38	0.61	3.5
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	20	3.28	0.39	3.34
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	20	2.95	0.67	2.74
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	20	2.79	0.46	2.86
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	20	2.79	0.83	2.63
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	20	2.55	0.5	2.54
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	20	2.35	0.46	2.45
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	20	2.1	0.33	2.1
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	20	1.46	0.26	1.43
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	19	2.81	0.82	2.84
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	19	2.77	0.75	2.71
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	19	2.38	0.69	2.52
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	19	1.9	0.4	1.71
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	19	1.82	0.42	1.92
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	18	2.17	0.74	1.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	17	2.2	1.02	2.04
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	17	1.84	0.75	1.64
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	17	1.58	0.29	1.62
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	16	2.81	0.88	2.92
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	16	2.42	0.75	2.44
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	16	2.14	0.6	1.98
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	15	3.45	1.1	3.32
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	15	2.54	1.45	2.05
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	15	1.77	0.35	1.72
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	15	1.42	0.27	1.45
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	14	2.43	0.74	2.54
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	14	1.44	0.24	1.42
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	13	2.1	0.6	2.15
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	13	1.75	0.38	1.75
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	13	1.58	0.7	1.45
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	13	1.57	0.49	1.42
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	12	1.51	0.5	1.36
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	12	1.49	0.34	1.43
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	11	1.94	0.84	1.63
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	11	1.66	0.46	1.5
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	11	1.42	0.24	1.39
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	10	2.63	0.41	2.5
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	10	1.62	0.36	1.68
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	10	1.6	0.41	1.52
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	10	1.58	0.39	1.44
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	9	1.73	0.42	1.68
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	9	1.67	0.32	1.63
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	8	2.86	1.48	2.78
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	8	2.01	0.87	1.78
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	8	1.62	0.47	1.48
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	8	1.58	0.33	1.58
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	8	1.35	0.21	1.28
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	8	1.25	0.15	1.27
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	7	2.14	1.11	2.04
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	7	2.02	0.72	1.9
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	7	1.82	0.67	1.91
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	7	1.64	0.69	1.31
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	7	1.59	0.5	1.53
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	7	1.53	0.4	1.34
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	7	1.5	0.28	1.6
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	7	1.27	0.14	1.31
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	6	1.49	0.23	1.46
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	6	1.4	0.44	1.24
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	6	1.26	0.11	1.23
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	5	1.87	1.28	1.36
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	5	1.73	0.34	1.73
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	5	1.72	0.4	1.53
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	5	1.51	0.27	1.44
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	5	1.37	0.21	1.47
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	5	1.29	0.38	1.16
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	5	1.18	0.22	1.07

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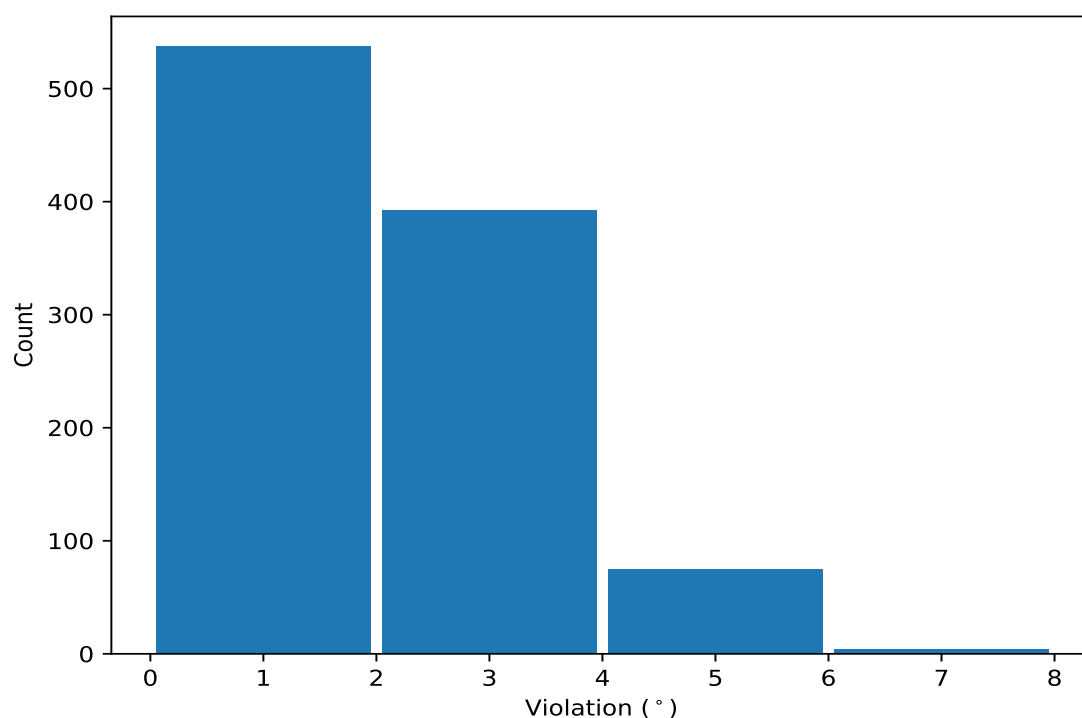
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,271)	1:154:A:ARG:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	4	1.96	0.85	1.86
(1,41)	1:26:A:LYS:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	4	1.68	0.33	1.56
(1,161)	1:88:A:LYS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	4	1.67	1.04	1.11
(1,197)	1:106:A:GLN:C	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	4	1.5	0.26	1.54
(1,277)	1:157:A:THR:C	1:158:A:TYR:N	1:158:A:TYR:CA	1:158:A:TYR:C	4	1.44	0.11	1.47
(1,311)	1:175:A:VAL:C	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	4	1.28	0.09	1.29
(1,228)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:ASP:N	3	3.32	0.2	3.25
(1,198)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLU:N	3	1.86	0.66	1.9
(1,322)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:VAL:N	3	1.72	0.36	1.66
(1,323)	1:183:A:SER:C	1:184:A:VAL:N	1:184:A:VAL:CA	1:184:A:VAL:C	3	1.68	0.12	1.65
(1,209)	1:112:A:ARG:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	3	1.61	0.34	1.65
(1,244)	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	1:134:A:LEU:N	3	1.48	0.13	1.5
(1,59)	1:35:A:GLN:C	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	3	1.45	0.18	1.49
(1,243)	1:132:A:GLN:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	3	1.42	0.28	1.49
(1,330)	1:187:A:VAL:N	1:187:A:VAL:CA	1:187:A:VAL:C	1:188:A:PHE:N	3	1.4	0.26	1.52
(1,155)	1:85:A:MET:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	3	1.26	0.05	1.24
(1,314)	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	1:178:A:VAL:N	3	1.19	0.11	1.2
(1,208)	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	1:113:A:ARG:N	3	1.16	0.12	1.1
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	2	1.74	0.13	1.74
(1,189)	1:102:A:ARG:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	2	1.42	0.06	1.42
(1,346)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ASP:N	2	1.38	0.06	1.38
(1,25)	1:18:A:VAL:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	2	1.34	0.12	1.34
(1,144)	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	1:81:A:LEU:N	2	1.31	0.22	1.31
(1,235)	1:128:A:GLU:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	2	1.31	0.02	1.31
(1,257)	1:147:A:ASN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	2	1.3	0.3	1.3
(1,31)	1:21:A:GLY:C	1:22:A:PRO:N	1:22:A:PRO:CA	1:22:A:PRO:C	2	1.28	0.08	1.28
(1,143)	1:79:A:ASP:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	2	1.23	0.19	1.23
(1,151)	1:83:A:ASP:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	2	1.18	0.18	1.18
(1,28)	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	1:21:A:GLY:N	2	1.09	0.04	1.09
(1,18)	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	1:16:A:ILE:N	2	1.08	0.05	1.08
(1,279)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	2	1.07	0.0	1.07
(1,258)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:GLU:N	2	1.06	0.05	1.06

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	15	6.62
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	20	6.49
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	1	6.35
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	20	6.05
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	3	5.66
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	20	5.65
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	13	5.64
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	7	5.63
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	3	5.62
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	2	5.61
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	10	5.52
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	5	5.46
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	3	5.42
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	14	5.38
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	12	5.36
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	10	5.33
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	17	5.3
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	18	5.3
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	5	5.22
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	7	5.21
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	8	5.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	20	5.15
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	9	5.14
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	9	5.14
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	7	5.07
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	16	5.05
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	14	5.04
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	19	5.03
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	11	4.89
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	17	4.8
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	11	4.77
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	4	4.73
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	3	4.7
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	4	4.7
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	6	4.7
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	20	4.65
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	18	4.55
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	9	4.55
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	5	4.53
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	19	4.51
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	16	4.49
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	12	4.47
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	9	4.44
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	12	4.41
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	15	4.41
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	14	4.37
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	7	4.37
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	7	4.35
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	15	4.33
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	19	4.33
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	12	4.31
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	13	4.3
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1	4.3
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	18	4.28
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	3	4.28
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	2	4.27
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	19	4.27
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	12	4.26
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	5	4.24
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	19	4.23
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	3	4.23
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1	4.23
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	1	4.23
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	7	4.22
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	1	4.16
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	20	4.15
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	11	4.15
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	15	4.14
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	10	4.11
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	14	4.11
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	17	4.11
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	2	4.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	3	4.09
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	16	4.07
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	17	4.04
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	6	4.03
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	7	4.03
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	8	4.02
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	2	4.01
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	17	3.99
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	10	3.98
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	1	3.97
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	12	3.97
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	14	3.95
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	19	3.95
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	12	3.95
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	2	3.94
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	8	3.92
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	3	3.92
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	2	3.86
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	4	3.85
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	18	3.82
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	13	3.8
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	14	3.8
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	13	3.77
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	4	3.75
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	19	3.75
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	6	3.74
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	8	3.71
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	10	3.7
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	12	3.69
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	7	3.68
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	3	3.67
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	12	3.65
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	5	3.63
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	10	3.62
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	17	3.61
(1,228)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:ASP:N	8	3.6
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	9	3.6
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	9	3.59
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	2	3.58
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	11	3.58
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	16	3.58
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	14	3.58
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	19	3.57
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	20	3.57
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	18	3.56
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	15	3.56
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	14	3.55
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	15	3.55
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	12	3.54
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	3	3.54
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	8	3.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	9	3.52
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	8	3.51
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	13	3.5
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	5	3.49
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	17	3.49
(1,161)	1:88:A:LYS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	16	3.47
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	8	3.47
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	4	3.46
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	13	3.46
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	14	3.46
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	6	3.45
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	13	3.45
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	14	3.43
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	15	3.42
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	18	3.42
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	16	3.41
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	10	3.39
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	13	3.39
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	4	3.38
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	16	3.37
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	4	3.37
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	11	3.37
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	4	3.36
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	4	3.36
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	13	3.36
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	19	3.36
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	16	3.35
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	5	3.35
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	7	3.35
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	18	3.34
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	18	3.33
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	1	3.33
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	17	3.33
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	19	3.33
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	9	3.33
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	2	3.33
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	13	3.32
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	3	3.32
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	16	3.32
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	10	3.31
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	10	3.3
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	13	3.29
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	2	3.29
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	4	3.29
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	5	3.29
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	9	3.28
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:ARG:N	18	3.28
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	19	3.28
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	9	3.27
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	4	3.27
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	20	3.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	15	3.26
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	12	3.26
(1,228)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:ASP:N	4	3.25
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	2	3.25
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	8	3.24
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	6	3.23
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	1	3.22
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	18	3.2
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	13	3.2
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	16	3.19
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	11	3.18
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	1	3.17
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	16	3.17
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	4	3.17
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	7	3.15
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	5	3.15
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	20	3.15
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	7	3.14
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	4	3.14
(1,228)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:ASP:N	11	3.12
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	15	3.11
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	8	3.11
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	11	3.11
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	7	3.11
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	10	3.11
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	6	3.08
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	1	3.08
(1,271)	1:154:A:ARG:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	14	3.07
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	13	3.07
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	7	3.07
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	18	3.07
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	2	3.06
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	19	3.05
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	10	3.04
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	10	3.04
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	19	3.04
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	17	3.03
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	8	3.02
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	7	3.01
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1	3.01
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	14	3.0
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	20	3.0
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	19	3.0
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	3	2.99
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	10	2.99
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	6	2.99
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	9	2.98
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	8	2.97
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	5	2.97
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	15	2.95
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	1	2.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	2	2.94
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	5	2.94
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	6	2.94
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	11	2.93
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	10	2.93
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	14	2.92
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	8	2.91
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	18	2.9
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	9	2.9
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	3	2.89
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	16	2.89
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	14	2.88
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	9	2.88
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	3	2.88
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	16	2.88
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	9	2.88
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	16	2.87
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	20	2.86
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	6	2.86
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	16	2.86
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	8	2.86
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	18	2.86
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	16	2.85
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	2	2.85
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	18	2.85
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	14	2.84
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	13	2.84
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	11	2.84
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	18	2.84
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	7	2.83
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	11	2.83
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	13	2.82
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	5	2.82
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	15	2.82
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	6	2.81
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	11	2.8
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	16	2.79
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	2	2.79
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	9	2.79
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	6	2.78
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	2	2.77
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	7	2.75
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	15	2.75
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	9	2.75
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	16	2.73
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	10	2.71
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	15	2.71
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	1	2.7
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	6	2.7
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	16	2.69
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	15	2.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	13	2.69
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	16	2.69
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	11	2.68
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	20	2.68
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	18	2.68
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	17	2.68
(1,84)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:ARG:N	15	2.68
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	12	2.68
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	11	2.66
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	18	2.65
(1,198)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLU:N	15	2.65
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	12	2.65
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	8	2.65
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	17	2.64
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	3	2.63
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	7	2.63
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	16	2.63
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	7	2.62
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	9	2.62
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	16	2.62
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	12	2.61
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	10	2.61
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	3	2.6
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	12	2.6
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	8	2.58
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	7	2.58
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	6	2.58
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	20	2.58
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	20	2.58
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	17	2.57
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	8	2.57
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	9	2.57
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	8	2.56
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	11	2.56
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	13	2.55
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	6	2.55
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	8	2.54
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	6	2.54
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	13	2.54
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	2	2.54
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	15	2.53
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	16	2.53
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	3	2.53
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	2	2.53
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	20	2.53
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	16	2.53
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	6	2.52
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	12	2.52
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	15	2.52
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	10	2.51
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	5	2.51

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,233)	1:127:A:PRO:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	7	2.5
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	2	2.5
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	17	2.5
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	15	2.49
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	12	2.49
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	5	2.49
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	16	2.49
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	13	2.49
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	14	2.49
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	17	2.48
(1,271)	1:154:A:ARG:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	2	2.48
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	3	2.48
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	14	2.48
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1	2.47
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	11	2.46
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	4	2.46
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1	2.46
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	10	2.46
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	8	2.45
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	3	2.45
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	10	2.45
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	1	2.44
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	2	2.44
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	11	2.43
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	17	2.43
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	9	2.42
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	3	2.41
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	17	2.41
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	3	2.41
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	7	2.41
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	7	2.41
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	14	2.41
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	5	2.4
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	15	2.4
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	5	2.4
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	19	2.39
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	9	2.38
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	20	2.38
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	17	2.37
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	7	2.37
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	13	2.36
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	14	2.36
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	15	2.36
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	13	2.36
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	3	2.36
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	1	2.36
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	10	2.35
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	10	2.35
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	19	2.35
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	1	2.34
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	14	2.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	14	2.34
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	2	2.33
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	9	2.33
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	18	2.33
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	17	2.33
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	7	2.32
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	17	2.32
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	16	2.32
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	19	2.32
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	8	2.32
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	12	2.32
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	4	2.32
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	14	2.31
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	13	2.3
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	8	2.3
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	20	2.3
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	20	2.28
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	15	2.28
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	2	2.28
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	9	2.27
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	5	2.27
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	3	2.27
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	4	2.26
(1,22)	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1:18:A:VAL:N	19	2.26
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	5	2.25
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	13	2.25
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	6	2.24
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	11	2.24
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	19	2.24
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	1	2.24
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	10	2.23
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	16	2.23
(1,343)	1:193:A:THR:C	1:194:A:HIS:N	1:194:A:HIS:CA	1:194:A:HIS:C	8	2.22
(1,176)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:ILE:N	12	2.22
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	5	2.22
(1,41)	1:26:A:LYS:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	18	2.22
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	7	2.21
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	3	2.21
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	2	2.21
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	9	2.2
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	7	2.2
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	10	2.2
(1,322)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:VAL:N	8	2.19
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	8	2.19
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	14	2.19
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	11	2.18
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	6	2.18
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	11	2.17
(1,102)	1:59:A:GLY:N	1:59:A:GLY:CA	1:59:A:GLY:C	1:60:A:LYS:N	15	2.17
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	16	2.16
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	14	2.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,316)	1:178:A:VAL:N	1:178:A:VAL:CA	1:178:A:VAL:C	1:179:A:ASN:N	18	2.15
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	20	2.15
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	4	2.15
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	20	2.14
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	15	2.14
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	2	2.13
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	19	2.13
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	4	2.13
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	17	2.12
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	13	2.12
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	8	2.12
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	6	2.11
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	11	2.11
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	11	2.11
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	15	2.11
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	20	2.1
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	2	2.1
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	2	2.1
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	9	2.1
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	16	2.1
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	8	2.09
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	8	2.09
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	20	2.09
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	7	2.08
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	14	2.05
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	9	2.05
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	7	2.05
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	16	2.05
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	9	2.04
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	14	2.04
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	9	2.04
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	10	2.04
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	6	2.03
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	4	2.03
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	1	2.03
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	19	2.03
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	18	2.02
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	17	2.01
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	16	2.0
(1,209)	1:112:A:ARG:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	7	2.0
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	2	2.0
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	12	2.0
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	5	1.99
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	12	1.99
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	7	1.99
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	4	1.99
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	20	1.99
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	11	1.98
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	12	1.97
(1,129)	1:72:A:VAL:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	11	1.97
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	17	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	9	1.96
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	19	1.96
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	2	1.95
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	6	1.94
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	14	1.93
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	15	1.93
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	7	1.93
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	13	1.92
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	6	1.92
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	13	1.92
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	4	1.91
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	3	1.91
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	10	1.91
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	5	1.91
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	15	1.9
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	2	1.9
(1,281)	1:159:A:TYR:C	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	16	1.9
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	20	1.9
(1,198)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLU:N	3	1.9
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	11	1.9
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	1	1.9
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	2	1.9
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	3	1.9
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	20	1.9
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	20	1.89
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	13	1.89
(1,231)	1:126:A:GLY:C	1:127:A:PRO:N	1:127:A:PRO:CA	1:127:A:PRO:C	11	1.89
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	13	1.89
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	11	1.89
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	17	1.88
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	9	1.88
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	10	1.88
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	19	1.88
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	8	1.88
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	18	1.87
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	19	1.87
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	4	1.87
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	5	1.87
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	7	1.86
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	16	1.86
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	20	1.86
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	10	1.85
(1,323)	1:183:A:SER:C	1:184:A:VAL:N	1:184:A:VAL:CA	1:184:A:VAL:C	14	1.85
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	18	1.85
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	10	1.84
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	20	1.84
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	17	1.84
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	18	1.84
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	19	1.83
(1,219)	1:118:A:THR:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	1	1.83
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	11	1.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	13	1.83
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	2	1.83
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	17	1.83
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	4	1.82
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	12	1.82
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	4	1.82
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	6	1.82
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	1	1.82
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	15	1.81
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	18	1.81
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	7	1.81
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	3	1.81
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	19	1.81
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	9	1.8
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	19	1.8
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	9	1.8
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	13	1.8
(1,197)	1:106:A:GLN:C	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	10	1.8
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	11	1.8
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	18	1.79
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	10	1.79
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	13	1.79
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	19	1.78
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	8	1.78
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	12	1.77
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	4	1.77
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	18	1.77
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	2	1.77
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	12	1.77
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	10	1.76
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1	1.76
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	20	1.76
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	11	1.76
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	1	1.75
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	14	1.75
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	5	1.75
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	17	1.75
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	19	1.75
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	10	1.75
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	12	1.74
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	2	1.74
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	3	1.73
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	17	1.73
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	12	1.73
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	20	1.73
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	6	1.72
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	9	1.72
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	10	1.72
(1,243)	1:132:A:GLN:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	14	1.72
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	10	1.72
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	9	1.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	11	1.72
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	15	1.71
(1,252)	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	1:138:A:GLY:N	14	1.71
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	18	1.71
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	14	1.71
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	1	1.71
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	20	1.7
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	19	1.69
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	13	1.69
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	17	1.69
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	13	1.69
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1	1.68
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	8	1.68
(1,197)	1:106:A:GLN:C	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1	1.68
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	17	1.68
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	19	1.68
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	20	1.67
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	2	1.67
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	18	1.67
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	11	1.67
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	15	1.67
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	7	1.67
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	18	1.67
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	19	1.67
(1,41)	1:26:A:LYS:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	10	1.67
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	19	1.67
(1,322)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:VAL:N	16	1.66
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	5	1.66
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	7	1.66
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	5	1.66
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	14	1.66
(1,330)	1:187:A:VAL:N	1:187:A:VAL:CA	1:187:A:VAL:C	1:188:A:PHE:N	18	1.65
(1,323)	1:183:A:SER:C	1:184:A:VAL:N	1:184:A:VAL:CA	1:184:A:VAL:C	16	1.65
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	19	1.65
(1,209)	1:112:A:ARG:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	2	1.65
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	13	1.65
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	8	1.65
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	17	1.65
(1,59)	1:35:A:GLN:C	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	9	1.65
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	2	1.65
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	17	1.64
(1,226)	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1:123:A:VAL:N	2	1.64
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	15	1.64
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	4	1.64
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	8	1.63
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	16	1.63
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	18	1.63
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	16	1.63
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	4	1.63
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	3	1.63
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	8	1.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	13	1.63
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	16	1.63
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	18	1.62
(1,244)	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	1:134:A:LEU:N	14	1.62
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	7	1.62
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	19	1.62
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	12	1.62
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	12	1.62
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	8	1.61
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	4	1.61
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	18	1.61
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	16	1.61
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	12	1.61
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	18	1.61
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	17	1.61
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	6	1.61
(1,257)	1:147:A:ASN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	18	1.6
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	4	1.6
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	19	1.6
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	19	1.59
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	12	1.59
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	18	1.59
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	5	1.58
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	2	1.58
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	10	1.58
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	14	1.58
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	7	1.58
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	20	1.58
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	4	1.57
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	13	1.57
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	7	1.57
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	3	1.56
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	2	1.56
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	20	1.56
(1,323)	1:183:A:SER:C	1:184:A:VAL:N	1:184:A:VAL:CA	1:184:A:VAL:C	8	1.55
(1,277)	1:157:A:THR:C	1:158:A:TYR:N	1:158:A:TYR:CA	1:158:A:TYR:C	17	1.55
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	16	1.55
(1,76)	1:44:A:THR:N	1:44:A:THR:CA	1:44:A:THR:C	1:45:A:GLY:N	11	1.55
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	9	1.55
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	4	1.54
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	18	1.54
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	2	1.53
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	2	1.53
(1,221)	1:119:A:LEU:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	12	1.53
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	14	1.53
(1,144)	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	1:81:A:LEU:N	3	1.53
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	5	1.53
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	15	1.53
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	20	1.53
(1,330)	1:187:A:VAL:N	1:187:A:VAL:CA	1:187:A:VAL:C	1:188:A:PHE:N	2	1.52
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	9	1.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	9	1.52
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	4	1.52
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	10	1.52
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	5	1.51
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	18	1.51
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	14	1.51
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1	1.5
(1,277)	1:157:A:THR:C	1:158:A:TYR:N	1:158:A:TYR:CA	1:158:A:TYR:C	10	1.5
(1,244)	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	1:134:A:LEU:N	10	1.5
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	3	1.5
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	16	1.49
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	12	1.49
(1,243)	1:132:A:GLN:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	7	1.49
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	8	1.49
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	13	1.49
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	7	1.49
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	19	1.49
(1,59)	1:35:A:GLN:C	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	16	1.49
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	6	1.48
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	7	1.48
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	15	1.48
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	15	1.48
(1,189)	1:102:A:ARG:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	8	1.48
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	17	1.48
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1	1.48
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	1	1.47
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	20	1.47
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	19	1.47
(1,73)	1:42:A:LEU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	17	1.47
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	7	1.47
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	11	1.46
(1,89)	1:50:A:SER:C	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	3	1.46
(1,25)	1:18:A:VAL:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	18	1.46
(1,346)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ASP:N	7	1.45
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	13	1.45
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	6	1.45
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	9	1.45
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	1	1.45
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	8	1.45
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	9	1.44
(1,277)	1:157:A:THR:C	1:158:A:TYR:N	1:158:A:TYR:CA	1:158:A:TYR:C	18	1.44
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	14	1.44
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	17	1.44
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	8	1.44
(1,41)	1:26:A:LYS:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	6	1.44
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	17	1.44
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	4	1.43
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	8	1.43
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	14	1.43
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	5	1.43
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	15	1.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	17	1.43
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	19	1.43
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	20	1.42
(1,143)	1:79:A:ASP:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	6	1.42
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	15	1.41
(1,196)	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	1:107:A:GLY:N	16	1.41
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	3	1.41
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	18	1.41
(1,311)	1:175:A:VAL:C	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	14	1.4
(1,197)	1:106:A:GLN:C	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	18	1.4
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	6	1.4
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	8	1.39
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	7	1.39
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	20	1.39
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	15	1.39
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	7	1.39
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	3	1.39
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	5	1.39
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	4	1.39
(1,41)	1:26:A:LYS:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	12	1.39
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	11	1.38
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	16	1.38
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	4	1.38
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	8	1.38
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	5	1.37
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	4	1.37
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	1	1.37
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	10	1.37
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	3	1.37
(1,56)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLN:N	18	1.37
(1,335)	1:189:A:SER:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	20	1.36
(1,189)	1:102:A:ARG:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	16	1.36
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	17	1.36
(1,31)	1:21:A:GLY:C	1:22:A:PRO:N	1:22:A:PRO:CA	1:22:A:PRO:C	17	1.36
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	16	1.35
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	4	1.35
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	9	1.35
(1,151)	1:83:A:ASP:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	16	1.35
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	10	1.35
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	18	1.35
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	17	1.35
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	19	1.35
(1,270)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:LEU:N	6	1.34
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	7	1.34
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	15	1.34
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	5	1.34
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	16	1.34
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	11	1.34
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	15	1.34
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	5	1.34
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	9	1.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,208)	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	1:113:A:ARG:N	10	1.33
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	2	1.33
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	3	1.33
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	20	1.33
(1,155)	1:85:A:MET:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	8	1.33
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	12	1.33
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	4	1.33
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	12	1.33
(1,17)	1:14:A:LYS:C	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	10	1.33
(1,346)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ASP:N	5	1.32
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	16	1.32
(1,314)	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	1:178:A:VAL:N	18	1.32
(1,311)	1:175:A:VAL:C	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	11	1.32
(1,235)	1:128:A:GLU:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	19	1.32
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	4	1.32
(1,349)	1:196:A:ASP:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	1	1.31
(1,322)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:VAL:N	14	1.31
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	9	1.31
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	20	1.31
(1,244)	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	1:134:A:LEU:N	16	1.31
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	11	1.31
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	5	1.31
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	5	1.31
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	2	1.31
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	3	1.3
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	16	1.3
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	12	1.3
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	19	1.3
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	16	1.3
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	10	1.29
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	17	1.29
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	3	1.29
(1,235)	1:128:A:GLU:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	14	1.29
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	10	1.29
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	17	1.28
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	2	1.28
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	5	1.28
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	11	1.28
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	6	1.28
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	14	1.28
(1,268)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:ARG:N	6	1.27
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	11	1.27
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	14	1.27
(1,5)	1:8:A:GLU:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	18	1.27
(1,311)	1:175:A:VAL:C	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	8	1.26
(1,277)	1:157:A:THR:C	1:158:A:TYR:N	1:158:A:TYR:CA	1:158:A:TYR:C	1	1.26
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	2	1.26
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	4	1.26
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	11	1.26
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	9	1.25
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	14	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	18	1.25
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	9	1.25
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	5	1.25
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	17	1.25
(1,240)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	5	1.24
(1,155)	1:85:A:MET:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	5	1.24
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	3	1.24
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	9	1.24
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	2	1.23
(1,271)	1:154:A:ARG:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	20	1.23
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	11	1.23
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	6	1.23
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	15	1.23
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	3	1.23
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	7	1.22
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	13	1.22
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	3	1.22
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	14	1.22
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	15	1.22
(1,105)	1:60:A:LYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	15	1.22
(1,59)	1:35:A:GLN:C	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	1	1.22
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	7	1.22
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	13	1.21
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	12	1.21
(1,161)	1:88:A:LYS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	7	1.21
(1,155)	1:85:A:MET:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	12	1.21
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	6	1.21
(1,124)	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1:71:A:LEU:N	12	1.21
(1,74)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:THR:N	17	1.21
(1,46)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:CYS:N	18	1.21
(1,31)	1:21:A:GLY:C	1:22:A:PRO:N	1:22:A:PRO:CA	1:22:A:PRO:C	11	1.21
(1,25)	1:18:A:VAL:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	1	1.21
(1,314)	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	1:178:A:VAL:N	4	1.2
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	19	1.2
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	20	1.2
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	6	1.19
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	9	1.19
(1,20)	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	1:17:A:PHE:N	19	1.19
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	6	1.18
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	3	1.18
(1,227)	1:122:A:TYR:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	6	1.18
(1,209)	1:112:A:ARG:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	9	1.18
(1,188)	1:102:A:ARG:N	1:102:A:ARG:CA	1:102:A:ARG:C	1:103:A:GLU:N	14	1.18
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	12	1.18
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	18	1.18
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	4	1.18
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1	1.18
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	3	1.17
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	3	1.17
(1,178)	1:97:A:ILE:N	1:97:A:ILE:CA	1:97:A:ILE:C	1:98:A:ASP:N	19	1.17
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	3	1.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	14	1.17
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	19	1.16
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	20	1.16
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	1	1.16
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	8	1.16
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	19	1.16
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	8	1.16
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	5	1.15
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	12	1.15
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	15	1.15
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	10	1.15
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	9	1.15
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	10	1.15
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	1	1.15
(1,87)	1:49:A:ARG:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	11	1.15
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	14	1.15
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	19	1.15
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	10	1.15
(1,311)	1:175:A:VAL:C	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	9	1.14
(1,245)	1:133:A:ARG:C	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	15	1.14
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	5	1.14
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	2	1.14
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	1	1.14
(1,49)	1:30:A:CYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	14	1.14
(1,18)	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	1:16:A:ILE:N	15	1.14
(1,16)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:ILE:N	9	1.14
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	17	1.13
(1,230)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ALA:N	10	1.13
(1,165)	1:90:A:ASN:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	17	1.13
(1,153)	1:84:A:ALA:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	4	1.13
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	17	1.13
(1,137)	1:76:A:THR:C	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	2	1.13
(1,55)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	20	1.13
(1,28)	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	1:21:A:GLY:N	5	1.13
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	4	1.12
(1,197)	1:106:A:GLN:C	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	6	1.12
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	9	1.12
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:MET:N	7	1.12
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	18	1.11
(1,166)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:SER:N	11	1.11
(1,159)	1:87:A:ALA:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	15	1.11
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	12	1.11
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1	1.11
(1,3)	1:7:A:GLU:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	13	1.11
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	6	1.1
(1,258)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:GLU:N	17	1.1
(1,208)	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	1:113:A:ARG:N	15	1.1
(1,131)	1:73:A:PRO:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	7	1.1
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	1	1.1
(1,52)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ILE:N	5	1.1
(1,342)	1:193:A:THR:N	1:193:A:THR:CA	1:193:A:THR:C	1:194:A:HIS:N	19	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	14	1.09
(1,312)	1:176:A:ARG:N	1:176:A:ARG:CA	1:176:A:ARG:C	1:177:A:LYS:N	16	1.09
(1,269)	1:153:A:LYS:C	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	14	1.09
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	4	1.09
(1,200)	1:108:A:GLU:N	1:108:A:GLU:CA	1:108:A:GLU:C	1:109:A:GLU:N	11	1.09
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	5	1.09
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	15	1.08
(1,172)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:PHE:N	15	1.08
(1,144)	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	1:81:A:LEU:N	19	1.08
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	20	1.08
(1,123)	1:69:A:GLY:C	1:70:A:GLN:N	1:70:A:GLN:CA	1:70:A:GLN:C	3	1.08
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1	1.08
(1,95)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	17	1.08
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	10	1.08
(1,67)	1:39:A:TYR:C	1:40:A:THR:N	1:40:A:THR:CA	1:40:A:THR:C	2	1.08
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	13	1.07
(1,279)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	17	1.07
(1,279)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	18	1.07
(1,185)	1:100:A:TYR:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	17	1.07
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	3	1.07
(1,109)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	8	1.07
(1,100)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:GLY:N	5	1.07
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	3	1.06
(1,314)	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	1:178:A:VAL:N	8	1.06
(1,208)	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	1:113:A:ARG:N	4	1.06
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ARG:N	11	1.06
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	15	1.06
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	19	1.06
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	11	1.06
(1,271)	1:154:A:ARG:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	9	1.05
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	19	1.05
(1,130)	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1:74:A:LEU:N	6	1.05
(1,79)	1:45:A:GLY:C	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	7	1.05
(1,43)	1:27:A:GLY:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	17	1.05
(1,28)	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	1:21:A:GLY:N	1	1.05
(1,332)	1:188:A:PHE:N	1:188:A:PHE:CA	1:188:A:PHE:C	1:189:A:SER:N	5	1.04
(1,330)	1:187:A:VAL:N	1:187:A:VAL:CA	1:187:A:VAL:C	1:188:A:PHE:N	4	1.04
(1,266)	1:152:A:LYS:N	1:152:A:LYS:CA	1:152:A:LYS:C	1:153:A:LYS:N	14	1.04
(1,243)	1:132:A:GLN:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	8	1.04
(1,182)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:TYR:N	1	1.04
(1,143)	1:79:A:ASP:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	17	1.04
(1,138)	1:77:A:VAL:N	1:77:A:VAL:CA	1:77:A:VAL:C	1:78:A:LEU:N	14	1.04
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	12	1.04
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	6	1.04
(1,111)	1:63:A:SER:C	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	10	1.04
(1,347)	1:195:A:LEU:C	1:196:A:ASP:N	1:196:A:ASP:CA	1:196:A:ASP:C	14	1.03
(1,318)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	19	1.03
(1,236)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:MET:N	12	1.03
(1,207)	1:111:A:GLU:C	1:112:A:ARG:N	1:112:A:ARG:CA	1:112:A:ARG:C	5	1.03
(1,198)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLU:N	19	1.03
(1,18)	1:15:A:ILE:N	1:15:A:ILE:CA	1:15:A:ILE:C	1:16:A:ILE:N	13	1.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,273)	1:155:A:LEU:C	1:156:A:GLU:N	1:156:A:GLU:CA	1:156:A:GLU:C	3	1.02
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	13	1.02
(1,173)	1:94:A:GLY:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	20	1.02
(1,126)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:VAL:N	18	1.02
(1,308)	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	1:174:A:ILE:N	11	1.01
(1,258)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:GLU:N	3	1.01
(1,250)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:ARG:N	2	1.01
(1,202)	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	1:110:A:PHE:N	11	1.01
(1,195)	1:105:A:GLN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	4	1.01
(1,161)	1:88:A:LYS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	17	1.01
(1,156)	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1:87:A:ALA:N	1	1.01
(1,135)	1:75:A:GLU:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	13	1.01
(1,127)	1:71:A:LEU:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	20	1.01
(1,257)	1:147:A:ASN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	15	1.0
(1,212)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:GLY:N	20	1.0
(1,161)	1:88:A:LYS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	5	1.0
(1,151)	1:83:A:ASP:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	15	1.0
(1,93)	1:52:A:VAL:C	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	20	1.0