



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 AM UTC

PDB ID : 2L4S / pdb_00002l4s
BMRB ID : 17254
Title : Promiscuous Binding at the Crossroads of Numerous Cancer Pathways: Insight from the Binding of GIP with Glutaminase L
Authors : Zoetewey, D.L.; Ovee, M.; Banerjee, M.; Bhaskaran, R.; Mohanty, S.
Deposited on : 2010-10-13

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

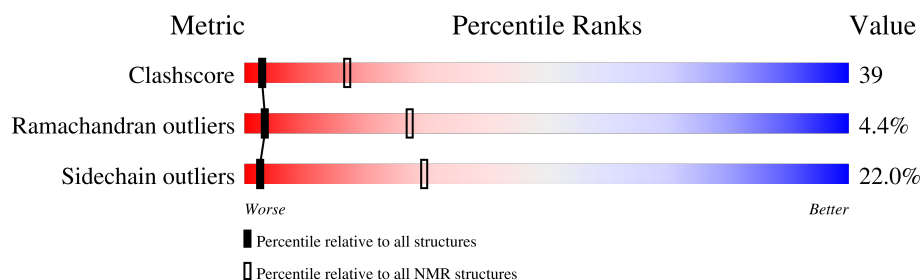
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	124	27% 40% 6% 27%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:10-A:39, A:54-A:114 (91)	0.64	4

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1946 atoms, of which 984 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tax1-binding protein 3.

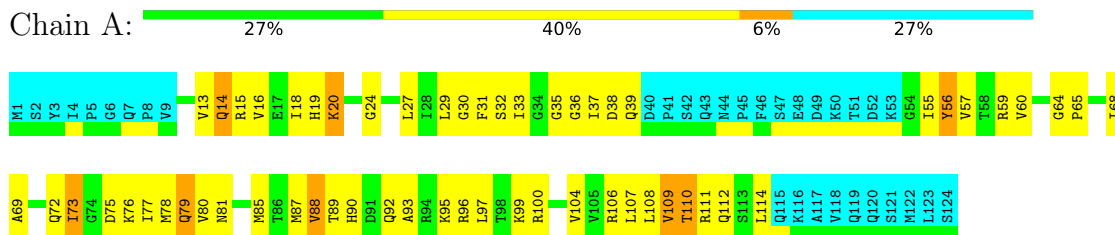
Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1946	596	984	175	186	5	

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: Tax1-binding protein 3

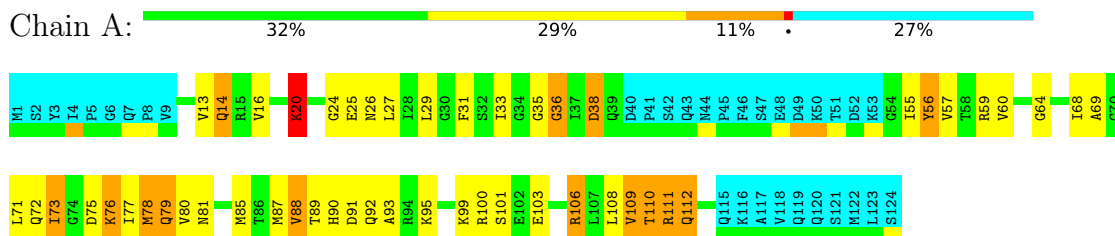


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

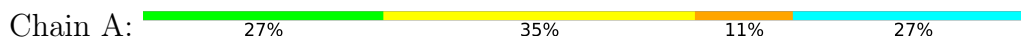
4.2.1 Score per residue for model 1

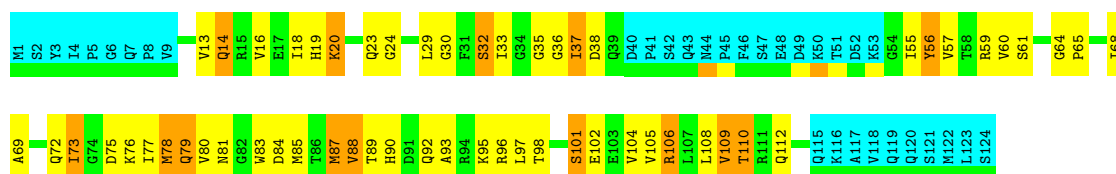
- Molecule 1: Tax1-binding protein 3

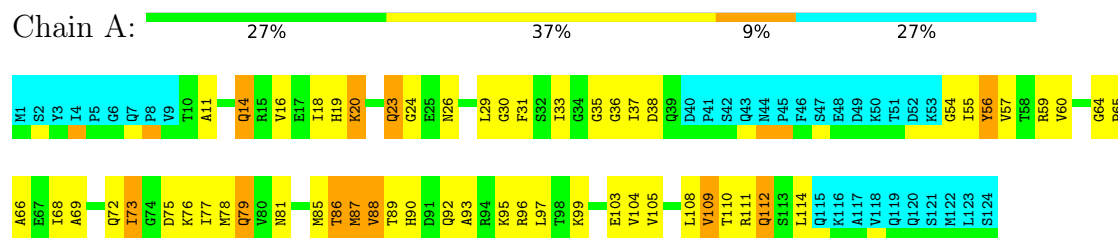


4.2.2 Score per residue for model 2

- Molecule 1: Tax1-binding protein 3

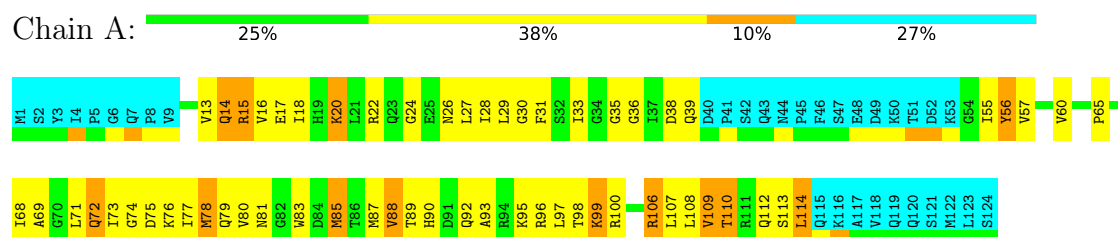






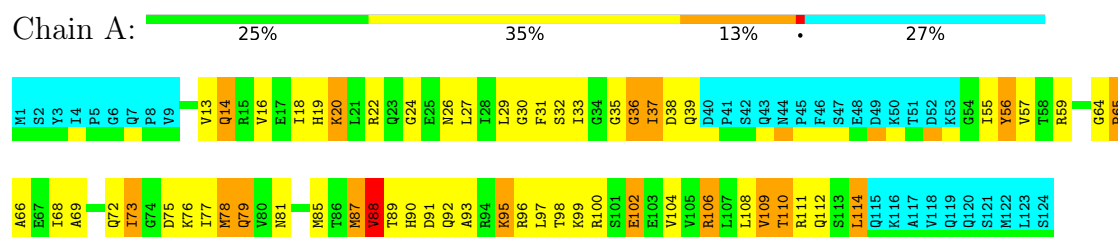
4.2.7 Score per residue for model 7

- Molecule 1: Tax1-binding protein 3



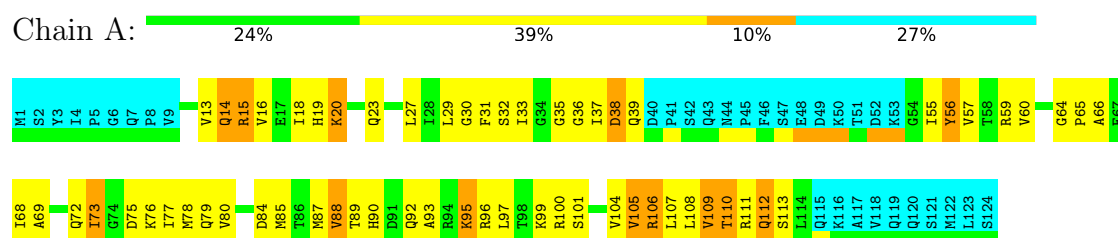
4.2.8 Score per residue for model 8

- Molecule 1: Tax1-binding protein 3



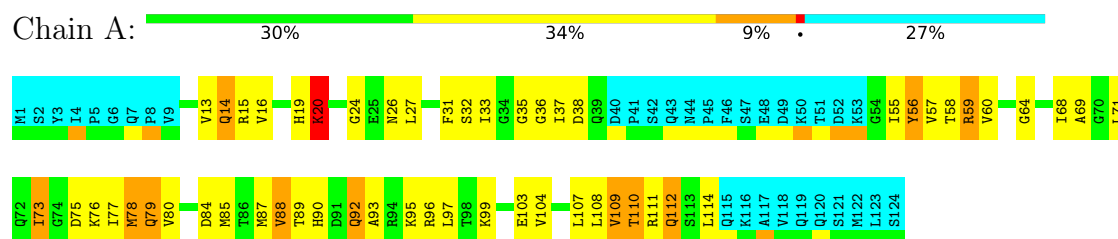
4.2.9 Score per residue for model 9

- Molecule 1: Tax1-binding protein 3



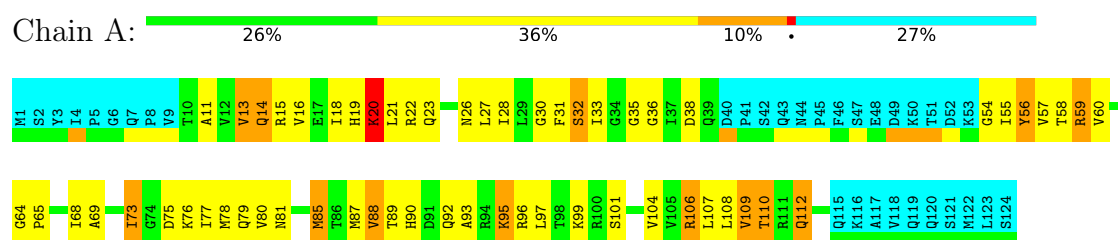
4.2.10 Score per residue for model 10

- Molecule 1: Tax1-binding protein 3



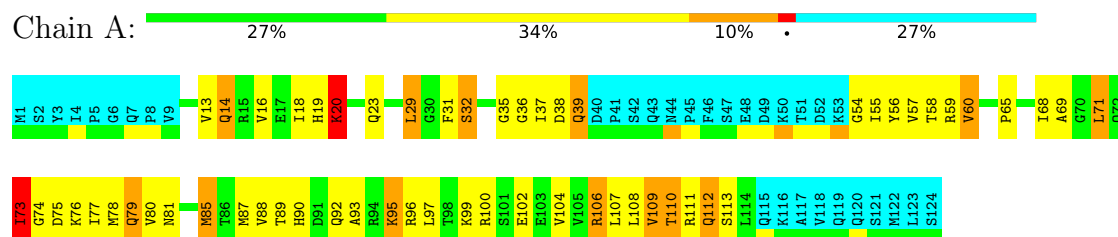
4.2.11 Score per residue for model 11

- Molecule 1: Tax1-binding protein 3



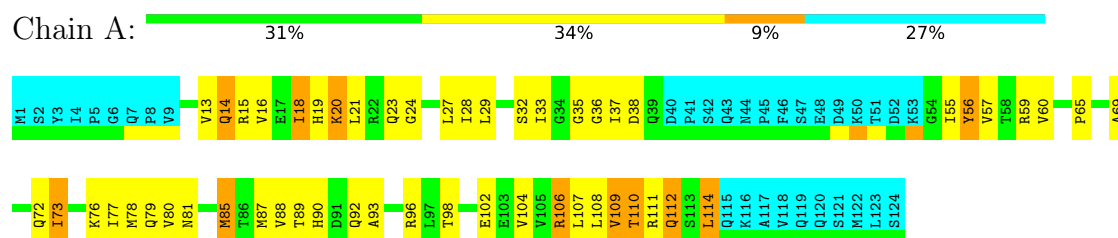
4.2.12 Score per residue for model 12

- Molecule 1: Tax1-binding protein 3



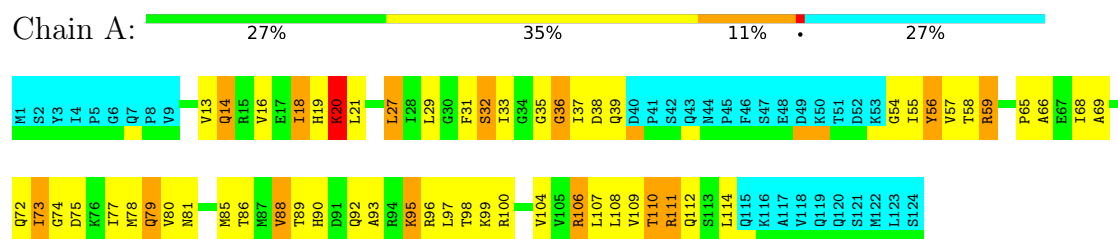
4.2.13 Score per residue for model 13

- Molecule 1: Tax1-binding protein 3



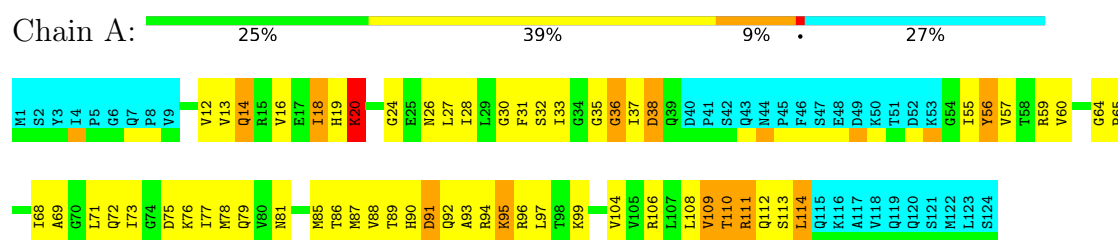
4.2.14 Score per residue for model 14

- Molecule 1: Tax1-binding protein 3



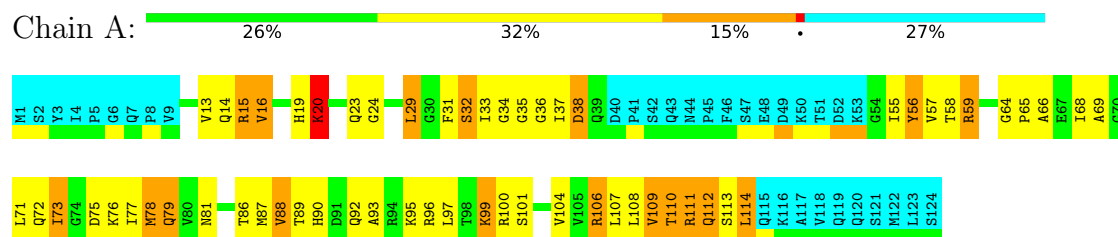
4.2.15 Score per residue for model 15

- Molecule 1: Tax1-binding protein 3



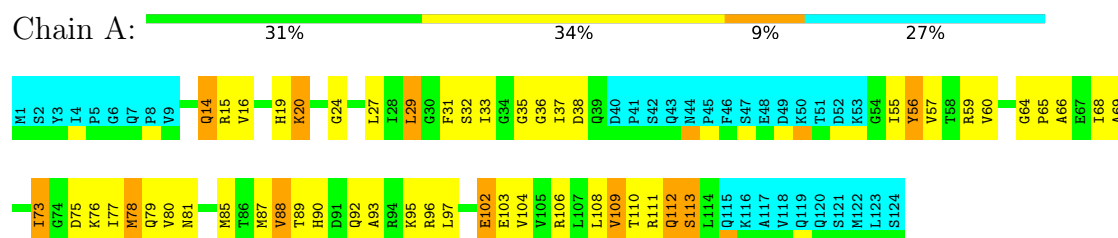
4.2.16 Score per residue for model 16

- Molecule 1: Tax1-binding protein 3



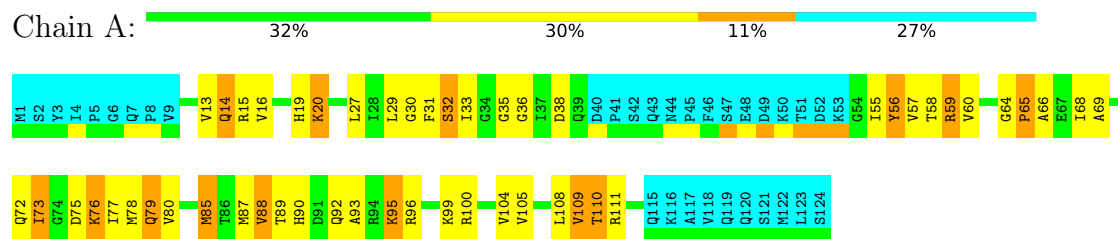
4.2.17 Score per residue for model 17

- Molecule 1: Tax1-binding protein 3



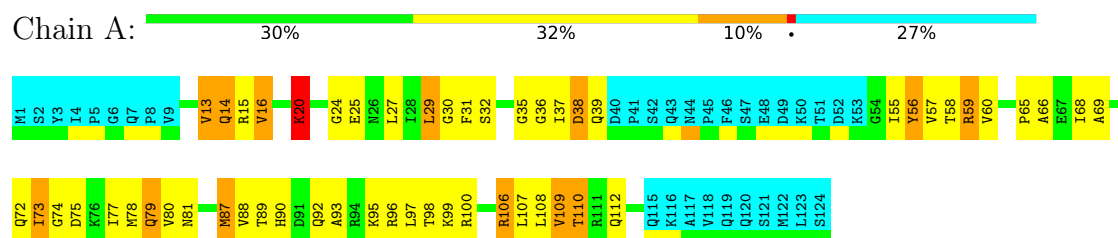
4.2.18 Score per residue for model 18

- Molecule 1: Tax1-binding protein 3



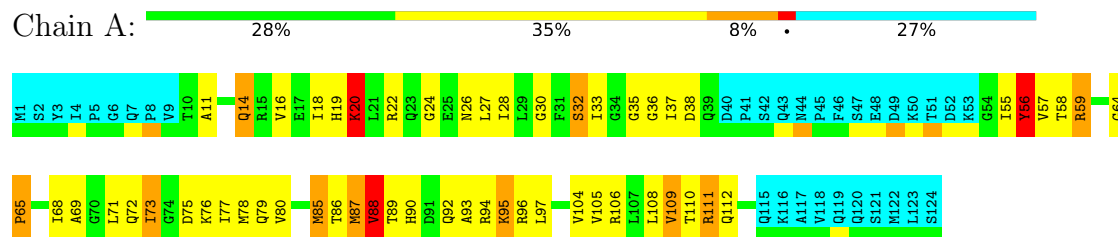
4.2.19 Score per residue for model 19

- Molecule 1: Tax1-binding protein 3



4.2.20 Score per residue for model 20

- Molecule 1: Tax1-binding protein 3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 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
ARIA	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1510
Number of shifts mapped to atoms	1510
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	0.70±0.03	0±0/712 (0.0± 0.0%)	0.90±0.02	0±0/958 (0.0± 0.0%)
All	All	0.70	0/14240 (0.0%)	0.90	1/19160 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.5
All	All	0	6

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	ILE	N-CA-C	-5.00	104.80	111.05	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	36	GLY	Peptide	5
1	A	56	TYR	Sidechain	1

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	705	735	733	57±5
All	All	14100	14700	14660	1135

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLY:HA3	1:A:55:ILE:HA	1.13	1.20	2	17
1:A:14:GLN:HE22	1:A:16:VAL:HG23	1.01	1.14	7	17
1:A:77:ILE:HG13	1:A:109:VAL:HG23	0.94	1.39	16	10
1:A:38:ASP:HB2	1:A:89:THR:HB	0.91	1.42	19	18
1:A:72:GLN:HB3	1:A:114:LEU:HB2	0.89	1.42	8	4
1:A:14:GLN:HG2	1:A:111:ARG:HD3	0.89	1.42	1	3
1:A:35:GLY:HA3	1:A:39:GLN:NE2	0.88	1.81	19	1
1:A:81:ASN:HA	1:A:106:ARG:HB2	0.84	1.47	13	11
1:A:16:VAL:HB	1:A:69:ALA:HB1	0.84	1.48	17	2
1:A:36:GLY:HA3	1:A:39:GLN:HG2	0.84	1.49	14	3
1:A:78:MET:HB2	1:A:108:LEU:HG	0.83	1.49	5	19
1:A:20:LYS:HB2	1:A:27:LEU:HD13	0.82	1.51	14	3
1:A:32:SER:HB3	1:A:58:THR:O	0.82	1.74	5	9
1:A:77:ILE:HG13	1:A:109:VAL:HG12	0.81	1.51	14	1
1:A:99:LYS:HA	1:A:99:LYS:HE2	0.81	1.51	1	2
1:A:59:ARG:HA	1:A:73:ILE:HG23	0.80	1.52	18	12
1:A:38:ASP:HB3	1:A:89:THR:HB	0.80	1.51	5	2
1:A:27:LEU:HD23	1:A:98:THR:HA	0.80	1.52	19	3
1:A:16:VAL:HB	1:A:107:LEU:HB3	0.79	1.52	7	4
1:A:78:MET:HA	1:A:78:MET:HE2	0.79	1.52	18	19
1:A:35:GLY:CA	1:A:55:ILE:HA	0.79	2.08	15	17
1:A:27:LEU:HD22	1:A:100:ARG:HA	0.79	1.53	9	2
1:A:14:GLN:HE22	1:A:16:VAL:HG13	0.79	1.35	17	1
1:A:19:HIS:HA	1:A:104:VAL:HA	0.77	1.55	8	14
1:A:13:VAL:HG12	1:A:110:THR:HG23	0.77	1.54	19	3
1:A:57:VAL:HG21	1:A:71:LEU:HD21	0.77	1.55	5	4
1:A:35:GLY:HA3	1:A:39:GLN:HE22	0.76	1.38	19	1
1:A:56:TYR:HB3	1:A:76:LYS:HA	0.76	1.57	2	12
1:A:30:GLY:HA3	1:A:65:PRO:HD2	0.76	1.58	8	11
1:A:56:TYR:HA	1:A:77:ILE:HD12	0.76	1.57	2	11
1:A:22:ARG:HA	1:A:27:LEU:HA	0.75	1.57	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLY:O	1:A:90:HIS:HA	0.74	1.83	13	17
1:A:38:ASP:HB3	1:A:89:THR:CB	0.73	2.13	12	2
1:A:38:ASP:HB2	1:A:89:THR:CB	0.73	2.13	20	18
1:A:92:GLN:O	1:A:96:ARG:HG2	0.71	1.85	11	15
1:A:27:LEU:HD13	1:A:100:ARG:HA	0.71	1.62	8	2
1:A:14:GLN:NE2	1:A:16:VAL:HG23	0.70	1.98	7	17
1:A:27:LEU:HD21	1:A:98:THR:HB	0.69	1.64	13	1
1:A:85:MET:SD	1:A:88:VAL:HG11	0.69	2.26	14	2
1:A:20:LYS:HE3	1:A:20:LYS:HA	0.69	1.64	18	4
1:A:80:VAL:HB	1:A:85:MET:HE3	0.69	1.65	3	1
1:A:55:ILE:HD13	1:A:85:MET:HB2	0.69	1.65	4	2
1:A:55:ILE:HG12	1:A:93:ALA:HB3	0.68	1.64	12	2
1:A:35:GLY:HA3	1:A:55:ILE:CA	0.68	2.12	1	16
1:A:16:VAL:HG13	1:A:69:ALA:CB	0.68	2.19	7	18
1:A:72:GLN:HG3	1:A:114:LEU:HB2	0.67	1.65	7	1
1:A:36:GLY:HA2	1:A:88:VAL:O	0.67	1.90	11	14
1:A:72:GLN:HE22	1:A:111:ARG:HB2	0.67	1.50	16	1
1:A:20:LYS:HB2	1:A:27:LEU:HD12	0.66	1.66	1	4
1:A:27:LEU:HD22	1:A:100:ARG:HG2	0.66	1.66	8	1
1:A:55:ILE:HD11	1:A:88:VAL:O	0.66	1.90	2	10
1:A:77:ILE:HG12	1:A:107:LEU:HD11	0.66	1.67	13	8
1:A:37:ILE:HG23	1:A:87:MET:O	0.66	1.91	12	2
1:A:35:GLY:O	1:A:55:ILE:HG13	0.66	1.91	7	15
1:A:29:LEU:H	1:A:29:LEU:HD23	0.66	1.50	19	3
1:A:38:ASP:HB3	1:A:90:HIS:H	0.66	1.49	19	17
1:A:35:GLY:HA3	1:A:55:ILE:HG13	0.65	1.68	14	3
1:A:36:GLY:N	1:A:39:GLN:HE22	0.65	1.88	5	2
1:A:80:VAL:HG21	1:A:97:LEU:HB3	0.65	1.66	2	2
1:A:57:VAL:HG12	1:A:75:ASP:H	0.65	1.50	10	14
1:A:13:VAL:HG22	1:A:110:THR:HG23	0.64	1.69	1	13
1:A:56:TYR:HB3	1:A:76:LYS:HD3	0.64	1.68	13	2
1:A:37:ILE:HG12	1:A:87:MET:O	0.64	1.93	2	3
1:A:55:ILE:HG22	1:A:77:ILE:HD13	0.64	1.70	13	5
1:A:77:ILE:HG13	1:A:109:VAL:CG2	0.63	2.22	7	1
1:A:20:LYS:HG2	1:A:105:VAL:HG21	0.63	1.71	6	3
1:A:18:ILE:HB	1:A:69:ALA:HB2	0.63	1.71	8	5
1:A:80:VAL:HG12	1:A:85:MET:SD	0.62	2.34	20	4
1:A:27:LEU:HB2	1:A:98:THR:HG23	0.62	1.71	7	1
1:A:14:GLN:HG3	1:A:109:VAL:HG12	0.62	1.71	17	17
1:A:57:VAL:HG23	1:A:77:ILE:HD11	0.62	1.71	13	1
1:A:35:GLY:C	1:A:39:GLN:HE22	0.62	2.01	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ILE:HG12	1:A:93:ALA:CB	0.61	2.24	11	15
1:A:21:LEU:HB3	1:A:28:ILE:HB	0.61	1.71	13	1
1:A:80:VAL:HB	1:A:85:MET:CE	0.61	2.26	3	3
1:A:29:LEU:HD13	1:A:98:THR:OG1	0.61	1.96	8	1
1:A:16:VAL:HG13	1:A:69:ALA:HB1	0.61	1.71	7	10
1:A:36:GLY:HA3	1:A:88:VAL:O	0.61	1.96	5	3
1:A:29:LEU:HD22	1:A:97:LEU:HD22	0.61	1.73	6	1
1:A:31:PHE:HD2	1:A:66:ALA:HB2	0.60	1.55	3	6
1:A:14:GLN:HG2	1:A:111:ARG:HD2	0.60	1.73	4	1
1:A:20:LYS:CE	1:A:27:LEU:HB3	0.60	2.26	9	1
1:A:18:ILE:HG13	1:A:65:PRO:O	0.60	1.96	14	3
1:A:96:ARG:O	1:A:99:LYS:HE2	0.60	1.96	16	3
1:A:14:GLN:CG	1:A:109:VAL:HG12	0.60	2.27	9	4
1:A:76:LYS:N	1:A:76:LYS:HD2	0.60	2.12	8	5
1:A:20:LYS:HG2	1:A:105:VAL:CG2	0.60	2.27	6	2
1:A:59:ARG:C	1:A:73:ILE:HA	0.59	2.23	6	10
1:A:13:VAL:HA	1:A:110:THR:HA	0.59	1.75	19	3
1:A:14:GLN:NE2	1:A:16:VAL:HG13	0.59	2.11	17	2
1:A:88:VAL:HB	1:A:92:GLN:HE21	0.59	1.57	13	1
1:A:72:GLN:HE22	1:A:111:ARG:HG3	0.59	1.58	3	7
1:A:14:GLN:HE21	1:A:109:VAL:HG12	0.59	1.58	16	1
1:A:59:ARG:O	1:A:60:VAL:HG23	0.58	1.97	17	7
1:A:16:VAL:HG13	1:A:69:ALA:HB3	0.58	1.75	18	9
1:A:57:VAL:HG11	1:A:71:LEU:HD22	0.57	1.74	10	1
1:A:29:LEU:HD11	1:A:97:LEU:HD21	0.57	1.75	8	1
1:A:55:ILE:HG22	1:A:77:ILE:HB	0.57	1.76	9	10
1:A:80:VAL:HG21	1:A:97:LEU:HB2	0.57	1.77	12	2
1:A:93:ALA:O	1:A:97:LEU:HG	0.57	2.00	11	3
1:A:78:MET:HE2	1:A:78:MET:CA	0.56	2.29	18	18
1:A:58:THR:HA	1:A:73:ILE:O	0.56	2.01	20	4
1:A:78:MET:HB2	1:A:108:LEU:CG	0.56	2.29	5	9
1:A:79:GLN:HB3	1:A:108:LEU:HD23	0.56	1.76	3	1
1:A:75:ASP:HB3	1:A:109:VAL:HG13	0.55	1.77	15	2
1:A:55:ILE:HG12	1:A:93:ALA:HB2	0.55	1.78	10	9
1:A:37:ILE:HD13	1:A:87:MET:O	0.55	2.02	5	2
1:A:58:THR:HG23	1:A:58:THR:O	0.55	2.02	14	1
1:A:95:LYS:O	1:A:99:LYS:HB3	0.55	2.02	18	1
1:A:25:GLU:HB3	1:A:100:ARG:HH11	0.55	1.61	19	1
1:A:31:PHE:HD1	1:A:66:ALA:HB2	0.54	1.61	19	2
1:A:20:LYS:HD3	1:A:27:LEU:HD12	0.54	1.80	8	1
1:A:29:LEU:HB2	1:A:31:PHE:CE2	0.54	2.38	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:CG	1:A:27:LEU:HD12	0.54	2.32	8	1
1:A:64:GLY:O	1:A:68:ILE:HD13	0.54	2.03	11	13
1:A:14:GLN:CD	1:A:109:VAL:HG12	0.54	2.27	7	2
1:A:99:LYS:HA	1:A:99:LYS:CE	0.54	2.23	9	2
1:A:79:GLN:HB2	1:A:84:ASP:HA	0.54	1.79	2	1
1:A:54:GLY:HA2	1:A:86:THR:O	0.54	2.03	6	2
1:A:20:LYS:HG2	1:A:102:GLU:O	0.54	2.02	13	3
1:A:72:GLN:HG2	1:A:72:GLN:O	0.54	2.03	7	1
1:A:80:VAL:HG22	1:A:85:MET:SD	0.54	2.43	11	1
1:A:22:ARG:HA	1:A:26:ASN:O	0.54	2.03	11	5
1:A:37:ILE:HG12	1:A:88:VAL:C	0.53	2.29	3	5
1:A:21:LEU:HD22	1:A:65:PRO:HD3	0.53	1.79	14	2
1:A:32:SER:HB2	1:A:59:ARG:HB2	0.53	1.79	2	3
1:A:59:ARG:O	1:A:73:ILE:HA	0.53	2.03	14	10
1:A:88:VAL:HG13	1:A:92:GLN:HG2	0.53	1.80	11	4
1:A:89:THR:OG1	1:A:92:GLN:HB2	0.53	2.04	13	2
1:A:72:GLN:HB2	1:A:75:ASP:OD2	0.53	2.04	1	3
1:A:14:GLN:HG2	1:A:111:ARG:CB	0.53	2.33	3	2
1:A:20:LYS:HA	1:A:20:LYS:CE	0.53	2.32	6	1
1:A:75:ASP:HB3	1:A:109:VAL:CG2	0.53	2.34	1	2
1:A:57:VAL:HG21	1:A:71:LEU:CD2	0.53	2.30	5	2
1:A:95:LYS:O	1:A:95:LYS:HE3	0.53	2.03	5	2
1:A:35:GLY:HA2	1:A:90:HIS:CG	0.52	2.39	5	2
1:A:15:ARG:NH1	1:A:17:GLU:HB2	0.52	2.19	7	1
1:A:99:LYS:HG2	1:A:102:GLU:OE1	0.52	2.04	8	1
1:A:95:LYS:HD3	1:A:95:LYS:C	0.52	2.29	10	9
1:A:79:GLN:HB3	1:A:108:LEU:HB3	0.52	1.80	3	13
1:A:29:LEU:HD13	1:A:97:LEU:HD21	0.52	1.81	5	2
1:A:85:MET:HE3	1:A:88:VAL:HG11	0.52	1.82	17	5
1:A:14:GLN:HG2	1:A:111:ARG:HB2	0.52	1.81	12	4
1:A:75:ASP:HB3	1:A:109:VAL:HG22	0.51	1.82	1	3
1:A:112:GLN:N	1:A:112:GLN:CD	0.51	2.67	6	3
1:A:57:VAL:O	1:A:74:GLY:HA2	0.51	2.05	12	3
1:A:72:GLN:O	1:A:73:ILE:HB	0.51	2.04	5	7
1:A:56:TYR:CA	1:A:77:ILE:HD12	0.51	2.35	18	8
1:A:20:LYS:HE2	1:A:27:LEU:HB3	0.51	1.81	9	1
1:A:80:VAL:HG12	1:A:85:MET:CE	0.51	2.35	17	4
1:A:55:ILE:O	1:A:77:ILE:N	0.51	2.44	2	16
1:A:14:GLN:O	1:A:109:VAL:HB	0.51	2.05	15	2
1:A:12:VAL:HG23	1:A:111:ARG:HG2	0.51	1.81	15	1
1:A:36:GLY:CA	1:A:39:GLN:HG2	0.50	2.31	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLY:HA2	1:A:54:GLY:O	0.50	2.06	12	1
1:A:55:ILE:HD13	1:A:85:MET:HB3	0.50	1.83	2	1
1:A:20:LYS:HG2	1:A:105:VAL:HG23	0.50	1.82	9	1
1:A:35:GLY:C	1:A:55:ILE:HG13	0.50	2.30	17	4
1:A:112:GLN:HE21	1:A:112:GLN:N	0.50	2.04	1	1
1:A:14:GLN:HG2	1:A:111:ARG:HB3	0.50	1.83	14	2
1:A:35:GLY:CA	1:A:55:ILE:HG13	0.49	2.37	14	2
1:A:68:ILE:HD12	1:A:68:ILE:N	0.49	2.22	19	12
1:A:56:TYR:HA	1:A:75:ASP:O	0.49	2.06	7	2
1:A:95:LYS:HE3	1:A:99:LYS:HD3	0.49	1.85	3	1
1:A:56:TYR:CB	1:A:76:LYS:HA	0.49	2.38	3	2
1:A:59:ARG:CA	1:A:73:ILE:HA	0.49	2.38	5	1
1:A:72:GLN:HG2	1:A:114:LEU:HD12	0.49	1.84	7	1
1:A:31:PHE:HB2	1:A:57:VAL:CG2	0.49	2.38	18	1
1:A:99:LYS:C	1:A:101:SER:H	0.49	2.15	1	4
1:A:20:LYS:CB	1:A:27:LEU:HD13	0.49	2.32	14	2
1:A:56:TYR:CD1	1:A:56:TYR:N	0.48	2.82	15	13
1:A:31:PHE:CZ	1:A:97:LEU:HD11	0.48	2.43	4	4
1:A:72:GLN:CB	1:A:114:LEU:HB2	0.48	2.33	3	1
1:A:89:THR:O	1:A:92:GLN:HB3	0.48	2.08	18	6
1:A:16:VAL:HG11	1:A:71:LEU:CD2	0.48	2.38	12	1
1:A:79:GLN:HB2	1:A:108:LEU:CB	0.48	2.39	13	1
1:A:77:ILE:HA	1:A:108:LEU:O	0.48	2.07	15	1
1:A:15:ARG:HD3	1:A:107:LEU:O	0.48	2.09	16	4
1:A:14:GLN:HE21	1:A:109:VAL:CG1	0.48	2.21	16	1
1:A:79:GLN:HB2	1:A:108:LEU:HB3	0.48	1.84	13	1
1:A:55:ILE:HD11	1:A:88:VAL:HG12	0.48	1.85	6	4
1:A:85:MET:CB	1:A:88:VAL:HB	0.48	2.39	8	1
1:A:75:ASP:OD1	1:A:111:ARG:HA	0.47	2.09	1	1
1:A:31:PHE:CD1	1:A:57:VAL:HG23	0.47	2.44	11	5
1:A:14:GLN:HG3	1:A:109:VAL:HG23	0.47	1.85	14	1
1:A:71:LEU:HD11	1:A:107:LEU:HD22	0.47	1.85	16	1
1:A:80:VAL:HG21	1:A:97:LEU:HG	0.47	1.84	19	1
1:A:88:VAL:HG13	1:A:92:GLN:HB3	0.47	1.86	8	8
1:A:20:LYS:HG3	1:A:102:GLU:HB2	0.47	1.87	2	1
1:A:32:SER:HB3	1:A:59:ARG:HB2	0.47	1.85	4	7
1:A:79:GLN:HA	1:A:85:MET:HG2	0.47	1.86	8	1
1:A:16:VAL:HG21	1:A:71:LEU:HG	0.47	1.85	16	2
1:A:75:ASP:OD2	1:A:111:ARG:HA	0.47	2.09	12	1
1:A:37:ILE:HG12	1:A:87:MET:C	0.47	2.34	2	1
1:A:98:THR:HG22	1:A:100:ARG:H	0.47	1.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:HD3	1:A:27:LEU:CD1	0.47	2.39	8	1
1:A:11:ALA:CB	1:A:112:GLN:HA	0.47	2.40	11	1
1:A:16:VAL:HG21	1:A:71:LEU:HD13	0.46	1.87	5	1
1:A:55:ILE:O	1:A:77:ILE:HB	0.46	2.08	12	2
1:A:32:SER:CB	1:A:59:ARG:HB2	0.46	2.41	4	5
1:A:38:ASP:HB2	1:A:89:THR:CA	0.46	2.40	13	1
1:A:58:THR:O	1:A:59:ARG:HG3	0.46	2.11	14	1
1:A:34:GLY:O	1:A:56:TYR:HD1	0.46	1.94	16	1
1:A:30:GLY:O	1:A:60:VAL:HA	0.46	2.11	18	1
1:A:112:GLN:H	1:A:112:GLN:CD	0.46	2.18	10	1
1:A:14:GLN:HG3	1:A:109:VAL:CG2	0.46	2.41	14	1
1:A:35:GLY:CA	1:A:90:HIS:HB2	0.46	2.41	19	3
1:A:112:GLN:CD	1:A:112:GLN:N	0.46	2.73	10	1
1:A:75:ASP:HB3	1:A:109:VAL:CG1	0.45	2.41	15	1
1:A:14:GLN:CG	1:A:111:ARG:HB2	0.45	2.41	20	1
1:A:20:LYS:CD	1:A:27:LEU:HD12	0.45	2.41	8	1
1:A:79:GLN:HA	1:A:85:MET:SD	0.45	2.51	12	1
1:A:31:PHE:HA	1:A:60:VAL:HA	0.45	1.88	1	6
1:A:35:GLY:O	1:A:90:HIS:CA	0.45	2.64	3	6
1:A:14:GLN:HE22	1:A:16:VAL:CG2	0.45	2.11	9	1
1:A:95:LYS:HD3	1:A:96:ARG:N	0.45	2.26	9	1
1:A:60:VAL:HG12	1:A:73:ILE:HD12	0.45	1.88	12	1
1:A:13:VAL:HG12	1:A:108:LEU:HD11	0.45	1.89	14	1
1:A:80:VAL:HG13	1:A:97:LEU:HB3	0.45	1.88	14	1
1:A:54:GLY:C	1:A:55:ILE:HD12	0.45	2.36	3	3
1:A:18:ILE:HD13	1:A:19:HIS:N	0.45	2.27	14	1
1:A:88:VAL:HG13	1:A:92:GLN:CG	0.45	2.42	16	2
1:A:38:ASP:HB3	1:A:89:THR:HA	0.44	1.88	15	1
1:A:37:ILE:HD11	1:A:88:VAL:HA	0.44	1.89	2	1
1:A:88:VAL:HG21	1:A:92:GLN:HE21	0.44	1.71	3	1
1:A:57:VAL:HG12	1:A:75:ASP:N	0.44	2.27	7	1
1:A:14:GLN:NE2	1:A:109:VAL:HG12	0.44	2.27	4	1
1:A:114:LEU:HD13	1:A:114:LEU:N	0.44	2.28	15	1
1:A:35:GLY:HA3	1:A:90:HIS:HB2	0.44	1.88	19	1
1:A:88:VAL:HG11	1:A:92:GLN:HG2	0.44	1.89	12	2
1:A:20:LYS:O	1:A:20:LYS:HD2	0.44	2.12	12	4
1:A:79:GLN:HG3	1:A:80:VAL:N	0.44	2.28	5	4
1:A:60:VAL:HG13	1:A:66:ALA:HB3	0.44	1.88	18	3
1:A:76:LYS:HE2	1:A:112:GLN:NE2	0.44	2.27	1	1
1:A:95:LYS:O	1:A:99:LYS:HG2	0.44	2.12	9	1
1:A:112:GLN:CD	1:A:114:LEU:HD21	0.44	2.38	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG12	1:A:65:PRO:HB2	0.44	1.90	4	8
1:A:11:ALA:HB1	1:A:111:ARG:O	0.44	2.13	20	2
1:A:101:SER:C	1:A:102:GLU:HG3	0.44	2.38	2	1
1:A:65:PRO:HA	1:A:68:ILE:HD13	0.43	1.90	19	2
1:A:78:MET:N	1:A:108:LEU:O	0.43	2.51	1	4
1:A:55:ILE:HG22	1:A:77:ILE:CD1	0.43	2.43	19	3
1:A:57:VAL:CG1	1:A:75:ASP:H	0.43	2.26	19	2
1:A:14:GLN:HG3	1:A:109:VAL:CG1	0.43	2.43	8	3
1:A:29:LEU:HD12	1:A:31:PHE:CE2	0.43	2.49	19	1
1:A:72:GLN:HB3	1:A:114:LEU:HB3	0.43	1.90	6	2
1:A:79:GLN:HB3	1:A:108:LEU:CB	0.43	2.44	12	2
1:A:85:MET:SD	1:A:85:MET:N	0.43	2.90	20	2
1:A:20:LYS:HB2	1:A:27:LEU:HB2	0.43	1.88	20	1
1:A:29:LEU:HD23	1:A:31:PHE:O	0.43	2.14	16	1
1:A:20:LYS:HD2	1:A:103:GLU:HA	0.43	1.90	1	1
1:A:106:ARG:CD	1:A:106:ARG:N	0.43	2.82	19	5
1:A:78:MET:HA	1:A:78:MET:CE	0.42	2.40	5	1
1:A:29:LEU:H	1:A:29:LEU:HD22	0.42	1.74	16	1
1:A:20:LYS:HB3	1:A:105:VAL:HG23	0.42	1.90	20	1
1:A:25:GLU:O	1:A:100:ARG:HD2	0.42	2.13	1	1
1:A:31:PHE:CE1	1:A:97:LEU:HD11	0.42	2.48	4	1
1:A:72:GLN:HB3	1:A:114:LEU:O	0.42	2.14	6	1
1:A:68:ILE:N	1:A:68:ILE:CD1	0.42	2.82	8	7
1:A:81:ASN:HD21	1:A:105:VAL:HG13	0.42	1.75	6	2
1:A:36:GLY:C	1:A:38:ASP:N	0.42	2.77	3	3
1:A:99:LYS:O	1:A:99:LYS:HG2	0.42	2.14	4	2
1:A:99:LYS:HB3	1:A:100:ARG:H	0.42	1.43	5	1
1:A:77:ILE:HA	1:A:109:VAL:HA	0.42	1.91	11	1
1:A:88:VAL:CB	1:A:92:GLN:HE21	0.42	2.27	13	1
1:A:18:ILE:HD12	1:A:65:PRO:HB2	0.42	1.90	14	1
1:A:83:TRP:HB2	1:A:85:MET:HE2	0.42	1.91	2	1
1:A:88:VAL:HG21	1:A:92:GLN:HG2	0.42	1.92	2	1
1:A:98:THR:HA	1:A:102:GLU:OE1	0.42	2.15	2	1
1:A:95:LYS:O	1:A:99:LYS:HB2	0.42	2.15	4	1
1:A:83:TRP:HB2	1:A:85:MET:HE1	0.42	1.89	7	1
1:A:77:ILE:CG1	1:A:109:VAL:HG23	0.42	2.45	9	1
1:A:29:LEU:O	1:A:66:ALA:HB2	0.42	2.15	16	1
1:A:21:LEU:HD22	1:A:64:GLY:HA2	0.42	1.92	11	1
1:A:75:ASP:HA	1:A:112:GLN:NE2	0.42	2.30	11	1
1:A:95:LYS:HD3	1:A:96:ARG:HD2	0.41	1.91	9	2
1:A:35:GLY:CA	1:A:90:HIS:CG	0.41	3.02	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ALA:O	1:A:97:LEU:HB2	0.41	2.15	19	2
1:A:112:GLN:CD	1:A:112:GLN:H	0.41	2.23	17	1
1:A:20:LYS:HE3	1:A:20:LYS:CA	0.41	2.40	6	1
1:A:88:VAL:CG1	1:A:92:GLN:HG2	0.41	2.45	2	1
1:A:85:MET:SD	1:A:88:VAL:CG1	0.41	3.09	3	1
1:A:14:GLN:N	1:A:109:VAL:O	0.41	2.54	5	1
1:A:37:ILE:HG23	1:A:87:MET:HA	0.41	1.93	6	1
1:A:72:GLN:O	1:A:74:GLY:N	0.41	2.54	7	1
1:A:112:GLN:HG2	1:A:113:SER:N	0.41	2.31	9	2
1:A:55:ILE:CD1	1:A:88:VAL:HG12	0.41	2.44	14	1
1:A:29:LEU:HD13	1:A:97:LEU:HD13	0.41	1.93	17	1
1:A:31:PHE:CD2	1:A:57:VAL:HG23	0.41	2.51	8	1
1:A:20:LYS:HD3	1:A:27:LEU:HG	0.41	1.92	17	1
1:A:58:THR:O	1:A:59:ARG:CB	0.41	2.69	5	2
1:A:30:GLY:CA	1:A:65:PRO:HD2	0.41	2.40	6	2
1:A:81:ASN:ND2	1:A:106:ARG:HH11	0.41	2.13	14	1
1:A:80:VAL:HG21	1:A:93:ALA:HB1	0.41	1.93	1	1
1:A:55:ILE:HD12	1:A:55:ILE:N	0.41	2.31	19	2
1:A:99:LYS:HE2	1:A:99:LYS:CA	0.41	2.36	9	1
1:A:80:VAL:HB	1:A:85:MET:HE2	0.41	1.92	14	1
1:A:20:LYS:HD3	1:A:20:LYS:O	0.41	2.16	3	1
1:A:13:VAL:CG1	1:A:108:LEU:HD11	0.41	2.46	4	1
1:A:38:ASP:HB2	1:A:89:THR:CG2	0.41	2.46	4	1
1:A:23:GLN:HB3	1:A:26:ASN:OD1	0.41	2.16	6	1
1:A:96:ARG:NE	1:A:96:ARG:HA	0.41	2.30	7	1
1:A:29:LEU:HD13	1:A:98:THR:HG1	0.41	1.75	8	1
1:A:91:ASP:CG	1:A:94:ARG:HH12	0.41	2.24	15	1
1:A:94:ARG:O	1:A:97:LEU:HG	0.41	2.15	20	1
1:A:60:VAL:HG12	1:A:61:SER:N	0.40	2.32	2	1
1:A:32:SER:O	1:A:57:VAL:HG23	0.40	2.15	19	1
1:A:112:GLN:OE1	1:A:114:LEU:HD23	0.40	2.16	10	1
1:A:57:VAL:HG21	1:A:71:LEU:HD12	0.40	1.93	12	1
1:A:97:LEU:HD12	1:A:98:THR:N	0.40	2.31	2	1
1:A:106:ARG:N	1:A:106:ARG:CD	0.40	2.85	11	2
1:A:79:GLN:N	1:A:108:LEU:HB3	0.40	2.31	13	1
1:A:114:LEU:H	1:A:114:LEU:HD22	0.40	1.75	16	1
1:A:76:LYS:N	1:A:76:LYS:CD	0.40	2.84	18	1
1:A:96:ARG:O	1:A:99:LYS:HG3	0.40	2.16	5	1
1:A:112:GLN:HG2	1:A:114:LEU:HD21	0.40	1.94	13	1
1:A:31:PHE:CD1	1:A:66:ALA:HB2	0.40	2.49	19	1
1:A:60:VAL:HG21	1:A:71:LEU:C	0.40	2.41	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LYS:HB2	1:A:99:LYS:HE3	0.40	1.60	12	1
1:A:38:ASP:HB3	1:A:90:HIS:N	0.40	2.29	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	91/124 (73%)	75±2 (83±2%)	12±2 (13±2%)	4±1 (4±1%)	3	27
All	All	1820/2480 (73%)	1503 (83%)	237 (13%)	80 (4%)	3	27

All 11 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	73	ILE	20
1	A	20	LYS	15
1	A	24	GLY	14
1	A	59	ARG	9
1	A	65	PRO	5
1	A	100	ARG	4
1	A	88	VAL	3
1	A	39	GLN	3
1	A	60	VAL	3
1	A	113	SER	3
1	A	102	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	76/107 (71%)	59±3 (78±4%)	17±3 (22±4%)	2	30
All	All	1520/2140 (71%)	1186 (78%)	334 (22%)	2	30

All 47 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	GLN	19
1	A	56	TYR	19
1	A	109	VAL	19
1	A	112	GLN	19
1	A	87	MET	18
1	A	110	THR	18
1	A	20	LYS	17
1	A	33	ILE	17
1	A	79	GLN	16
1	A	106	ARG	14
1	A	95	LYS	14
1	A	88	VAL	13
1	A	29	LEU	11
1	A	78	MET	10
1	A	23	GLN	8
1	A	85	MET	8
1	A	15	ARG	8
1	A	32	SER	7
1	A	99	LYS	7
1	A	111	ARG	6
1	A	114	LEU	6
1	A	86	THR	6
1	A	38	ASP	5
1	A	26	ASN	4
1	A	37	ILE	4
1	A	28	ILE	4
1	A	81	ASN	4
1	A	91	ASP	3
1	A	103	GLU	3
1	A	18	ILE	3
1	A	76	LYS	2
1	A	39	GLN	2
1	A	72	GLN	2
1	A	102	GLU	2
1	A	84	ASP	2
1	A	13	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	16	VAL	2
1	A	101	SER	1
1	A	10	THR	1
1	A	57	VAL	1
1	A	105	VAL	1
1	A	92	GLN	1
1	A	71	LEU	1
1	A	73	ILE	1
1	A	27	LEU	1
1	A	107	LEU	1
1	A	113	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1510
Number of shifts mapped to atoms	1510
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	124	0.00 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.32 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	123	-0.05 ± 0.08	None needed (< 0.5 ppm)
^{15}N	116	-0.40 ± 0.54	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1130 atoms were assigned a chemical shift out of a possible 1275. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	463/464 (100%)	192/192 (100%)	181/182 (99%)	90/90 (100%)
Sidechain	641/764 (84%)	452/497 (91%)	180/230 (78%)	9/37 (24%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	26/47 (55%)	14/23 (61%)	11/19 (58%)	1/5 (20%)
Overall	1130/1275 (89%)	658/712 (92%)	372/431 (86%)	100/132 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1510 atoms were assigned a chemical shift out of a possible 1700. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	617/622 (99%)	254/255 (100%)	247/248 (100%)	116/119 (97%)
Sidechain	861/1012 (85%)	605/656 (92%)	242/310 (78%)	14/46 (30%)
Aromatic	32/66 (48%)	18/32 (56%)	13/29 (45%)	1/5 (20%)
Overall	1510/1700 (89%)	877/943 (93%)	502/587 (86%)	131/170 (77%)

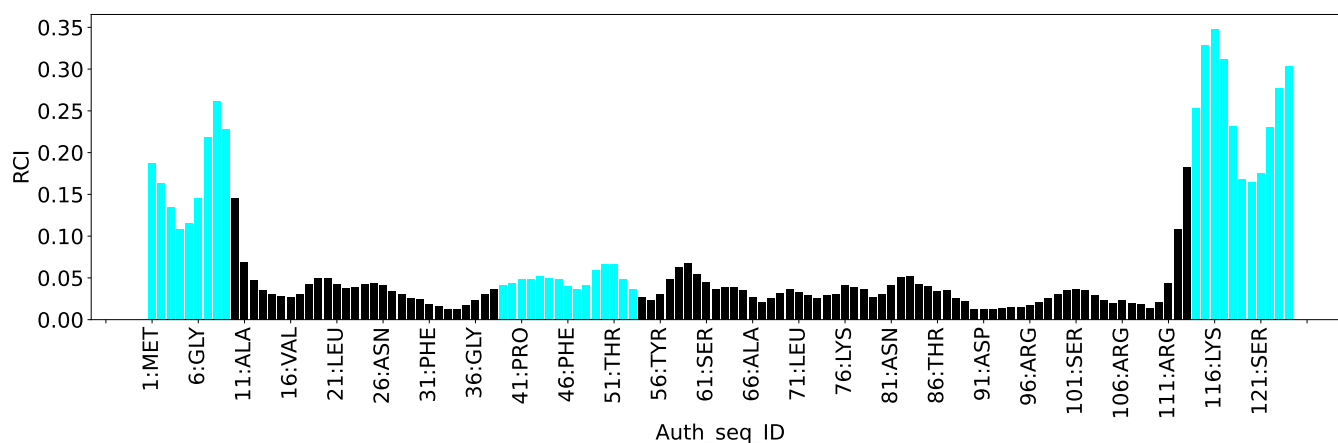
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3256
Intra-residue ($ i-j =0$)	1350
Sequential ($ i-j =1$)	873
Medium range ($ i-j >1$ and $ i-j <5$)	340
Long range ($ i-j \geq 5$)	629
Inter-chain	0
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	118
Number of unmapped restraints	0
Number of restraints per residue	27.2
Number of long range restraints per residue ¹	5.4

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)	87.7	0.2
0.2-0.5 (Medium)	59.3	0.5
>0.5 (Large)	52.2	3.08

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)	17.8	9.9
10.0-20.0 (Medium)	2.2	18.55
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

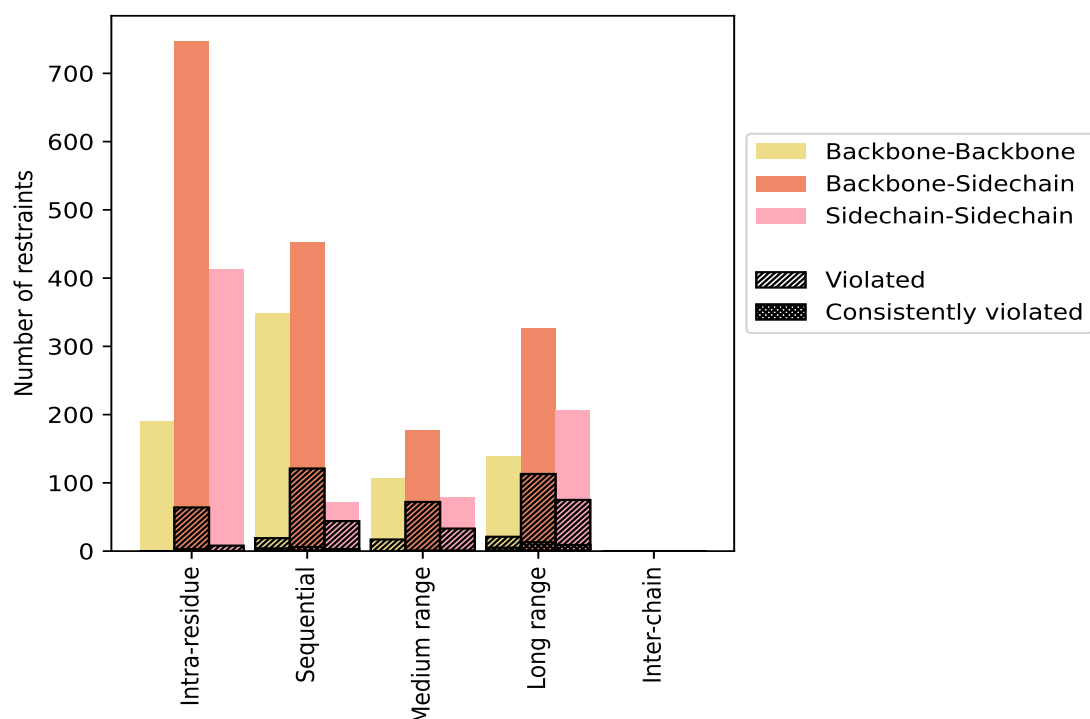
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1350	41.5	72	5.3	2.2	3	0.2	0.1
Backbone-Backbone	190	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	747	22.9	64	8.6	2.0	3	0.4	0.1
Sidechain-Sidechain	413	12.7	8	1.9	0.2	0	0.0	0.0
Sequential ($i-j =1$)	873	26.8	184	21.1	5.7	13	1.5	0.4
Backbone-Backbone	348	10.7	19	5.5	0.6	4	1.1	0.1
Backbone-Sidechain	453	13.9	121	26.7	3.7	6	1.3	0.2
Sidechain-Sidechain	72	2.2	44	61.1	1.4	3	4.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	340	10.4	120	35.3	3.7	2	0.6	0.1
Backbone-Backbone	107	3.3	17	15.9	0.5	0	0.0	0.0
Backbone-Sidechain	155	4.8	70	45.2	2.1	1	0.6	0.0
Sidechain-Sidechain	78	2.4	33	42.3	1.0	1	1.3	0.0
Long range ($i-j \geq 5$)	629	19.3	193	30.7	5.9	20	3.2	0.6
Backbone-Backbone	139	4.3	21	15.1	0.6	5	3.6	0.2
Backbone-Sidechain	284	8.7	97	34.2	3.0	6	2.1	0.2
Sidechain-Sidechain	206	6.3	75	36.4	2.3	9	4.4	0.3
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	64	2.0	18	28.1	0.6	7	10.9	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3256	100.0	587	18.0	18.0	45	1.4	1.4
Backbone-Backbone	784	24.1	57	7.3	1.8	9	1.1	0.3
Backbone-Sidechain	1703	52.3	370	21.7	11.4	23	1.4	0.7
Sidechain-Sidechain	769	23.6	160	20.8	4.9	13	1.7	0.4

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	20	70	27	71	0	188	0.44	2.63	0.45	0.22
2	25	71	31	79	0	206	0.41	3.08	0.48	0.2
3	23	65	31	79	0	198	0.43	2.62	0.45	0.22
4	18	65	26	72	0	181	0.44	2.69	0.48	0.24
5	19	64	33	88	0	204	0.45	2.15	0.47	0.22
6	20	66	37	75	0	198	0.43	2.75	0.47	0.22
7	21	77	35	92	0	225	0.45	2.46	0.47	0.24
8	15	73	34	77	0	199	0.44	2.68	0.48	0.22
9	20	69	29	77	0	195	0.41	2.7	0.46	0.21
10	22	67	35	76	0	200	0.41	1.67	0.38	0.23

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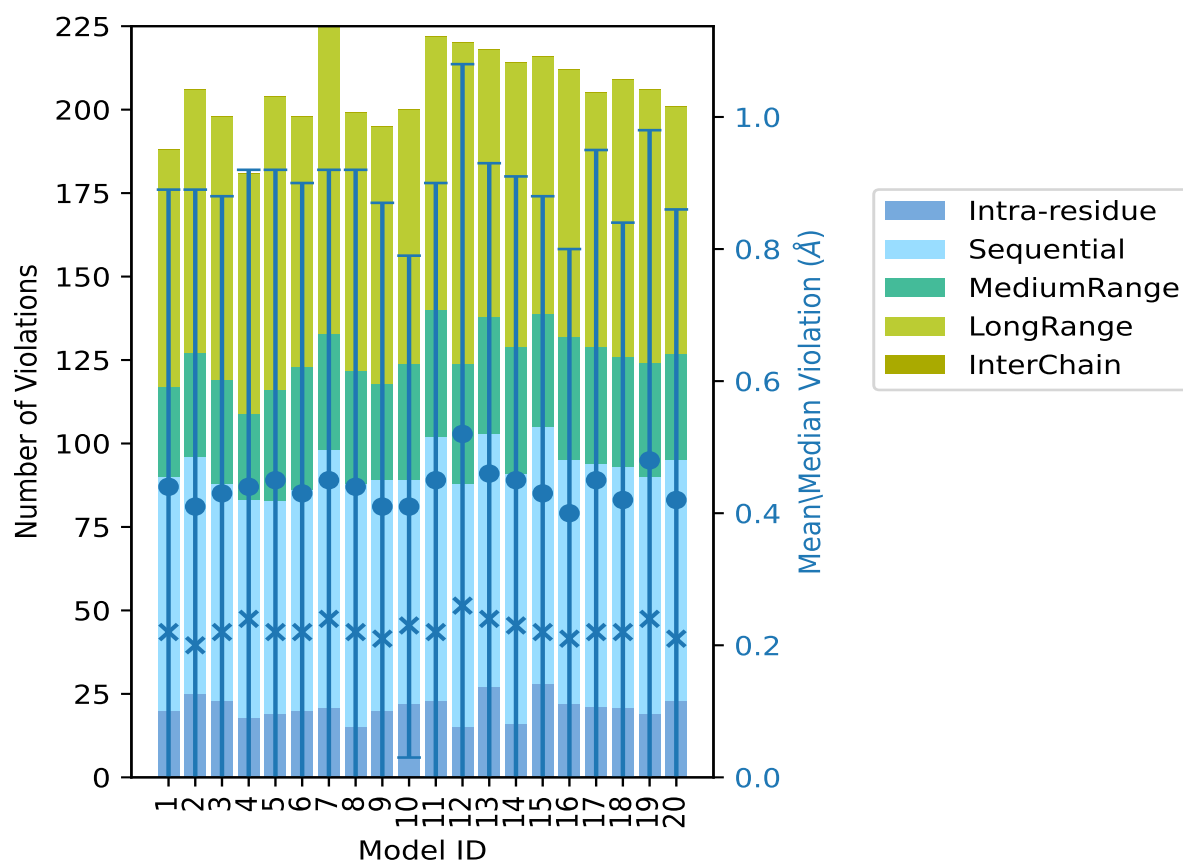
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	23	79	38	82	0	222	0.45	1.93	0.45	0.22
12	15	73	36	96	0	220	0.52	2.68	0.56	0.26
13	27	76	35	80	0	218	0.46	2.58	0.47	0.24
14	16	75	38	85	0	214	0.45	2.65	0.46	0.23
15	28	77	34	77	0	216	0.43	2.69	0.45	0.22
16	22	73	37	80	0	212	0.4	1.92	0.4	0.21
17	21	73	35	76	0	205	0.45	2.77	0.5	0.22
18	21	72	33	83	0	209	0.42	1.76	0.42	0.22
19	19	71	34	82	0	206	0.48	2.19	0.5	0.24
20	23	72	32	74	0	201	0.42	2.42	0.44	0.21

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

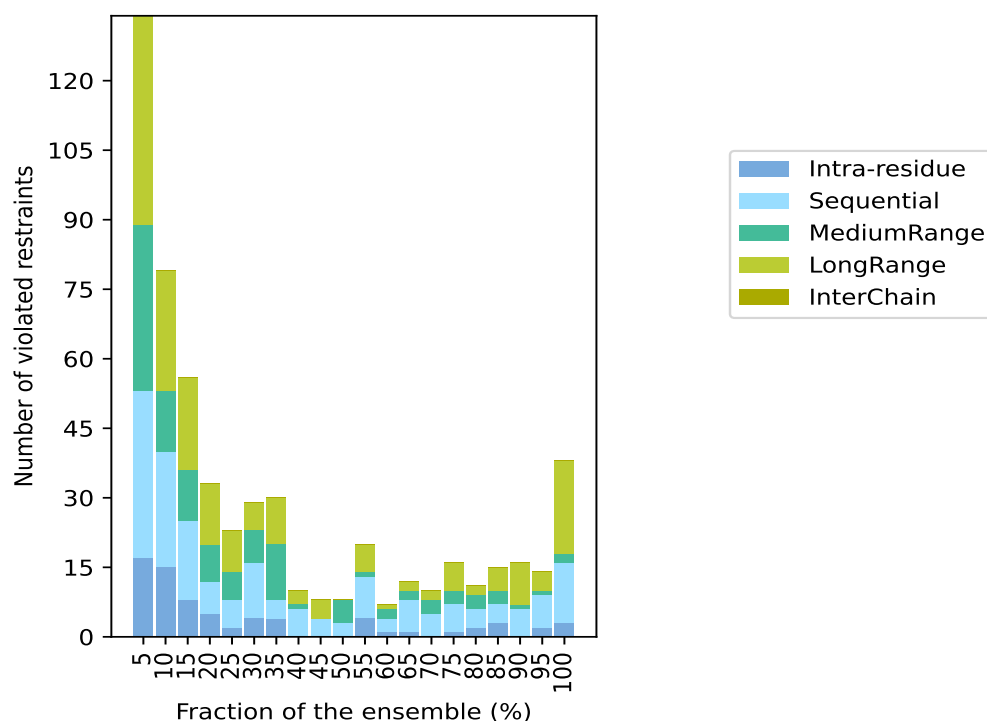
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2623(IR:1278, SQ:689, MR:220, LR:436, IC:0) restraints are 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	%
17	36	36	45	0	134	1	5.0
15	25	13	26	0	79	2	10.0
8	17	11	20	0	56	3	15.0
5	7	8	13	0	33	4	20.0
2	6	6	9	0	23	5	25.0
4	12	7	6	0	29	6	30.0
4	4	12	10	0	30	7	35.0
0	6	1	3	0	10	8	40.0
0	4	0	4	0	8	9	45.0
0	3	5	0	0	8	10	50.0
4	9	1	6	0	20	11	55.0
1	3	2	1	0	7	12	60.0
1	7	2	2	0	12	13	65.0
0	5	3	2	0	10	14	70.0
1	6	3	6	0	16	15	75.0
2	4	3	2	0	11	16	80.0
3	4	3	5	0	15	17	85.0
0	6	1	9	0	16	18	90.0
2	7	1	4	0	14	19	95.0
3	13	2	20	0	38	20	100.0

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

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

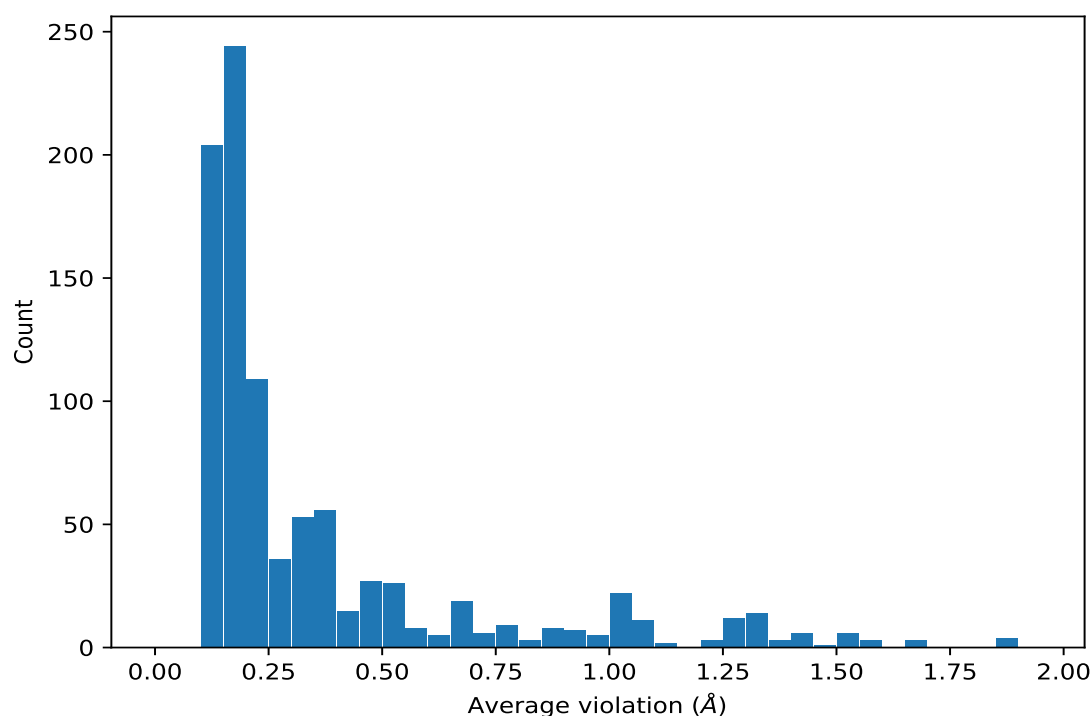
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,53)	1:32:A:SER:H	1:58:A:THR:O	20	1.87	0.92	2.52
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	20	1.51	0.2	1.48
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	20	1.5	0.08	1.5
(2,59)	1:32:A:SER:N	1:58:A:THR:O	20	1.49	1.01	2.22
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	20	1.39	0.21	1.42
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	20	1.35	0.12	1.35
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	20	1.33	0.12	1.31
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	20	1.31	0.11	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	20	1.31	0.11	1.34
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	20	1.3	0.2	1.32
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	20	1.28	0.46	1.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	20	1.22	0.44	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	20	1.22	0.44	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	20	1.22	0.44	1.42
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	20	1.11	0.51	1.06
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	20	1.03	0.44	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	20	1.03	0.44	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	20	1.03	0.44	1.23
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	20	1.02	0.42	1.17
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	20	1.02	0.42	1.17
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	20	1.02	0.06	1.02
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	20	1.02	0.06	1.02
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	20	1.02	0.06	1.02
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	20	1.01	0.81	0.32
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	20	1.01	0.81	0.32
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	20	1.01	0.81	0.32
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	20	0.99	0.74	1.55
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	20	0.96	0.03	0.97
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	20	0.77	0.23	0.74
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	20	0.77	0.23	0.74
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	20	0.77	0.23	0.74
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	20	0.76	0.09	0.76
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	20	0.73	0.57	0.66
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	20	0.73	0.57	0.66
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	20	0.73	0.57	0.66
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	20	0.68	0.19	0.76
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	20	0.64	0.26	0.72
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	20	0.58	0.54	0.4
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	20	0.53	0.31	0.49
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	20	0.53	0.16	0.48
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	20	0.5	0.46	0.34
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	20	0.48	0.55	0.32
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	20	0.48	0.55	0.32
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	20	0.48	0.55	0.32
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	20	0.47	0.21	0.45
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	20	0.46	0.55	0.18
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	20	0.45	0.03	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	20	0.45	0.03	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	20	0.45	0.03	0.44
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	20	0.45	0.57	0.22
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	20	0.37	0.12	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	20	0.37	0.12	0.38
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	20	0.37	0.12	0.38
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	20	0.36	0.02	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	20	0.36	0.02	0.37
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	20	0.33	0.05	0.35
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	20	0.32	0.09	0.36
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	20	0.31	0.15	0.28
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	20	0.22	0.05	0.21
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	20	0.21	0.05	0.22
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	20	0.21	0.05	0.22
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	20	0.21	0.05	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	20	0.21	0.05	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	20	0.21	0.05	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	20	0.21	0.05	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	20	0.21	0.05	0.2
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	20	0.21	0.05	0.2
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	20	0.21	0.05	0.2
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	20	0.21	0.03	0.21
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	20	0.21	0.03	0.21
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	20	0.21	0.03	0.21
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	20	0.2	0.02	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	20	0.2	0.04	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	20	0.2	0.04	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	20	0.2	0.04	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	20	0.18	0.03	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	20	0.18	0.03	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	20	0.18	0.03	0.17
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	20	0.17	0.04	0.18
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	19	1.06	0.27	1.09
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	19	0.54	0.13	0.61
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	19	0.46	0.09	0.44
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	19	0.45	0.03	0.46
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	19	0.44	0.13	0.51
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	19	0.38	0.41	0.25
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	19	0.37	0.12	0.37
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	19	0.37	0.12	0.37
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	19	0.37	0.12	0.37
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	19	0.32	0.04	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	19	0.32	0.04	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	19	0.32	0.04	0.3
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	19	0.31	0.2	0.23
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	19	0.31	0.2	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	19	0.31	0.2	0.23
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	19	0.26	0.11	0.21
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	19	0.26	0.11	0.21
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	19	0.26	0.11	0.21
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	19	0.25	0.07	0.25
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	19	0.2	0.03	0.2
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	19	0.19	0.04	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	19	0.15	0.03	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	19	0.15	0.03	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	19	0.15	0.03	0.16
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	19	0.11	0.01	0.11
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	18	1.54	0.22	1.58
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	18	1.54	0.22	1.58
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	18	1.54	0.22	1.58
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	18	1.4	0.32	1.48
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	18	1.05	0.45	1.26
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	18	0.94	0.17	0.92
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	18	0.94	0.17	0.92
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	18	0.94	0.17	0.92
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	18	0.68	0.52	0.5
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	18	0.61	0.09	0.58
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	18	0.54	0.11	0.52
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	18	0.54	0.11	0.52
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	18	0.54	0.11	0.52
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	18	0.38	0.13	0.37
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	18	0.37	0.6	0.15
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	18	0.36	0.14	0.37
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	18	0.36	0.14	0.37
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	18	0.34	0.08	0.36
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	18	0.27	0.05	0.26
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	18	0.19	0.03	0.19
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	18	0.19	0.05	0.18
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	18	0.19	0.05	0.18
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	18	0.19	0.05	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	18	0.17	0.02	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	18	0.17	0.02	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	18	0.17	0.02	0.17
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	18	0.16	0.04	0.15
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	17	1.33	0.52	1.16
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	17	1.06	0.11	1.09
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	17	0.99	0.52	0.82
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	17	0.85	0.44	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	17	0.5	0.23	0.55
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	17	0.25	0.06	0.25
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	17	0.25	0.06	0.25
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	17	0.25	0.06	0.25
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	17	0.23	0.03	0.23
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	17	0.22	0.05	0.21
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	17	0.22	0.07	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	17	0.22	0.07	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	17	0.22	0.07	0.2
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	17	0.22	0.08	0.23
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	17	0.22	0.08	0.23
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	17	0.19	0.04	0.2
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	17	0.19	0.04	0.2
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	17	0.18	0.03	0.18
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	17	0.17	0.05	0.17
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	17	0.17	0.05	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	17	0.15	0.03	0.15
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	17	0.15	0.03	0.15
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	17	0.15	0.02	0.15
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	17	0.13	0.02	0.13
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	17	0.13	0.02	0.13
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	17	0.13	0.02	0.13
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	16	0.86	0.54	1.23
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	16	0.86	0.54	1.23
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	16	0.86	0.54	1.23
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	16	0.5	0.23	0.51
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	16	0.34	0.23	0.27
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	16	0.18	0.11	0.14
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	16	0.18	0.04	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	16	0.18	0.04	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	16	0.18	0.04	0.18
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	16	0.18	0.06	0.16
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	16	0.17	0.05	0.16
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	16	0.17	0.05	0.16
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	16	0.16	0.04	0.14
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	16	0.15	0.04	0.15
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	16	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	16	0.11	0.01	0.11
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	15	1.42	0.36	1.44
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	15	1.4	0.36	1.42
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	15	0.79	0.37	0.7
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	15	0.49	0.32	0.43
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	15	0.33	0.57	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	15	0.33	0.57	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	15	0.33	0.57	0.17
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	15	0.26	0.07	0.27
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	15	0.2	0.04	0.2
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	15	0.2	0.04	0.2
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	15	0.19	0.07	0.19
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	15	0.19	0.07	0.19
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	15	0.19	0.07	0.19
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	15	0.18	0.06	0.16
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	15	0.18	0.06	0.16
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	15	0.18	0.06	0.16
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	15	0.17	0.06	0.15
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	15	0.17	0.06	0.15
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	15	0.17	0.06	0.15
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	15	0.17	0.04	0.17
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	15	0.17	0.04	0.19
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	15	0.17	0.04	0.19
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	15	0.17	0.03	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	15	0.17	0.03	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	15	0.17	0.03	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	15	0.16	0.01	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	15	0.15	0.03	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	15	0.15	0.03	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	15	0.15	0.03	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	15	0.15	0.03	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	15	0.15	0.03	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	15	0.15	0.03	0.15
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	14	1.07	0.06	1.06
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	14	0.66	0.45	0.48
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	14	0.43	0.45	0.26
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	14	0.34	0.64	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	14	0.34	0.64	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	14	0.34	0.64	0.16
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	14	0.18	0.02	0.18
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	14	0.18	0.02	0.18
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	14	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	14	0.15	0.02	0.15
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	14	0.15	0.06	0.12
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	14	0.15	0.02	0.15
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	14	0.13	0.02	0.12
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	14	0.12	0.02	0.12
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	13	0.95	0.29	0.96
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	13	0.52	0.43	0.36
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	13	0.5	0.65	0.17
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	13	0.37	0.59	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	13	0.37	0.59	0.22
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	13	0.35	0.17	0.32
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	13	0.35	0.17	0.32
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	13	0.34	0.16	0.36
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	13	0.32	0.16	0.28
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	13	0.26	0.03	0.27
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	13	0.18	0.05	0.18
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	13	0.13	0.03	0.12
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	13	0.13	0.03	0.12
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	13	0.13	0.03	0.12
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	13	0.13	0.02	0.12
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	13	0.11	0.01	0.11
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	12	0.91	0.74	0.98
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	12	0.79	0.43	0.78
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	12	0.58	0.77	0.16
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	12	0.58	0.77	0.16
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	12	0.58	0.77	0.16
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	12	0.4	0.14	0.46
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	12	0.39	0.18	0.34
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	12	0.33	0.14	0.35
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	12	0.17	0.06	0.15
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	12	0.15	0.04	0.14
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	11	1.07	0.26	0.98
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	11	0.95	0.42	0.93
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	11	0.65	0.24	0.75
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	11	0.48	0.45	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	11	0.48	0.45	0.27
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	11	0.46	0.35	0.34
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	11	0.34	0.14	0.35
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	11	0.34	0.14	0.35
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	11	0.34	0.14	0.35
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	11	0.28	0.09	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	11	0.28	0.09	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	11	0.28	0.09	0.29
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	11	0.2	0.04	0.19
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	11	0.19	0.07	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	11	0.17	0.06	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	11	0.17	0.06	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	11	0.17	0.06	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	11	0.17	0.06	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	11	0.17	0.06	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	11	0.17	0.06	0.16
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	11	0.15	0.04	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	11	0.15	0.04	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	11	0.15	0.04	0.15
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	11	0.15	0.02	0.15
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	11	0.15	0.02	0.15
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	11	0.14	0.02	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	11	0.14	0.02	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	11	0.14	0.02	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	11	0.14	0.03	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	11	0.14	0.03	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	11	0.14	0.03	0.14
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	11	0.14	0.03	0.13
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	11	0.14	0.03	0.13
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	11	0.14	0.03	0.13
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	11	0.14	0.03	0.13
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	11	0.14	0.03	0.13
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	11	0.14	0.03	0.13
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	11	0.14	0.02	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	11	0.14	0.01	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	11	0.14	0.01	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	11	0.14	0.01	0.14
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	11	0.13	0.02	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	11	0.13	0.02	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	11	0.13	0.02	0.13
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	11	0.12	0.02	0.12
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	10	0.54	0.29	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	10	0.39	0.14	0.39
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	10	0.39	0.14	0.39
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	10	0.39	0.14	0.39
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	10	0.37	0.09	0.38
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	10	0.37	0.09	0.38
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	10	0.37	0.09	0.38
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	10	0.23	0.08	0.24
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	10	0.18	0.04	0.18
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	10	0.18	0.06	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	10	0.18	0.06	0.16
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	10	0.14	0.04	0.13
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	10	0.13	0.03	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	10	0.13	0.03	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	10	0.13	0.03	0.12
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	9	0.51	0.44	0.38
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	9	0.51	0.44	0.38
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	9	0.51	0.44	0.38
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	9	0.47	0.22	0.48
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	9	0.47	0.22	0.48
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	9	0.47	0.22	0.48
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	9	0.35	0.16	0.38
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	9	0.35	0.16	0.38
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	9	0.35	0.16	0.38
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	9	0.28	0.06	0.31
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	9	0.21	0.05	0.22
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	9	0.16	0.05	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	9	0.16	0.05	0.14
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	9	0.16	0.03	0.16
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	9	0.16	0.03	0.16
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	9	0.16	0.03	0.16
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	9	0.15	0.05	0.14
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	9	0.15	0.05	0.14
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	9	0.15	0.05	0.14
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	9	0.15	0.05	0.14
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	9	0.15	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	9	0.15	0.05	0.14
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	8	0.5	0.17	0.44
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	8	0.42	0.2	0.54
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	8	0.41	0.25	0.39
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	8	0.41	0.25	0.39
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	8	0.41	0.25	0.39
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	8	0.25	0.03	0.24
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	8	0.23	0.08	0.22
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	8	0.22	0.07	0.2
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	8	0.19	0.09	0.15
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	8	0.14	0.04	0.12
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	8	0.14	0.04	0.12
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	8	0.14	0.04	0.12
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	8	0.13	0.02	0.13
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	8	0.13	0.02	0.13
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	8	0.12	0.02	0.11
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	7	1.14	0.1	1.11
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	7	0.8	0.46	0.85
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	7	0.58	0.11	0.62
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	7	0.51	0.18	0.54
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	7	0.4	0.15	0.34
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	7	0.38	0.26	0.28
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	7	0.38	0.26	0.28
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	7	0.38	0.26	0.28
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	7	0.38	0.22	0.45
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	7	0.34	0.25	0.14
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	7	0.34	0.25	0.14
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	7	0.32	0.07	0.32
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	7	0.22	0.12	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	7	0.22	0.12	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	7	0.22	0.12	0.15
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	7	0.21	0.02	0.2
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	7	0.2	0.06	0.21
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	7	0.2	0.06	0.21
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	7	0.2	0.06	0.21
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	7	0.2	0.08	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	7	0.2	0.01	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	7	0.2	0.01	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	7	0.2	0.01	0.2
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	7	0.2	0.05	0.19
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	7	0.19	0.06	0.16
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	7	0.19	0.06	0.16
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	7	0.19	0.06	0.21
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	7	0.19	0.06	0.21
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	7	0.19	0.06	0.21
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	7	0.19	0.07	0.17
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	7	0.19	0.07	0.17
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	7	0.18	0.06	0.16
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	7	0.18	0.08	0.15
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	7	0.18	0.08	0.15
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	7	0.16	0.04	0.17
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	7	0.16	0.04	0.17
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	7	0.16	0.04	0.17
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	7	0.15	0.03	0.16
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	7	0.15	0.03	0.15
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	7	0.15	0.04	0.14
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	7	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	7	0.15	0.03	0.15
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	7	0.14	0.02	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	7	0.14	0.02	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	7	0.14	0.02	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	7	0.14	0.02	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	7	0.14	0.02	0.13
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	7	0.13	0.03	0.12
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	7	0.13	0.03	0.12
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	7	0.13	0.03	0.12
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	7	0.12	0.01	0.12
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	6	0.69	0.12	0.74
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	6	0.69	0.12	0.74
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	6	0.56	0.2	0.56
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	6	0.56	0.2	0.56
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	6	0.56	0.2	0.56
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	6	0.49	0.38	0.26
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	6	0.43	0.37	0.26
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	6	0.4	0.51	0.22
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	6	0.38	0.19	0.42
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	6	0.38	0.19	0.42
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	6	0.38	0.19	0.42
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	6	0.38	0.19	0.42
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	6	0.38	0.19	0.42
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	6	0.38	0.19	0.42
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	6	0.34	0.12	0.34
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	6	0.29	0.36	0.14
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	6	0.27	0.09	0.3
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	6	0.25	0.05	0.29
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	6	0.24	0.1	0.22
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	6	0.22	0.09	0.21
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	6	0.21	0.1	0.2
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	6	0.2	0.07	0.18
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	6	0.19	0.09	0.15
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	6	0.19	0.09	0.15
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	6	0.18	0.1	0.12
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	6	0.18	0.1	0.12
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	6	0.18	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	6	0.17	0.05	0.16
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	6	0.16	0.02	0.17
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	6	0.16	0.03	0.16
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	6	0.16	0.04	0.15
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	6	0.16	0.04	0.15
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	6	0.16	0.04	0.15
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	6	0.16	0.04	0.15
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	6	0.16	0.04	0.15
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	6	0.16	0.04	0.15
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	6	0.14	0.04	0.14
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	6	0.14	0.03	0.13
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	6	0.14	0.03	0.13
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	6	0.14	0.03	0.13
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	6	0.14	0.03	0.13
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	6	0.14	0.03	0.13
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	6	0.14	0.03	0.12
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	6	0.14	0.03	0.12
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	6	0.13	0.01	0.14
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	6	0.13	0.04	0.12
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	6	0.13	0.04	0.12
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	6	0.13	0.01	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	6	0.13	0.01	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	6	0.13	0.01	0.13
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	6	0.13	0.02	0.13
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	6	0.12	0.02	0.12
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	6	0.12	0.02	0.12
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	6	0.12	0.02	0.12
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	6	0.12	0.01	0.12
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	5	1.35	0.25	1.28
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	5	1.01	0.24	1.15
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	5	0.38	0.11	0.39
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	5	0.38	0.11	0.39
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	5	0.38	0.11	0.39
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	5	0.35	0.4	0.15
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	5	0.35	0.4	0.15
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	5	0.35	0.4	0.15
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	5	0.34	0.11	0.31
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	5	0.27	0.07	0.26
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	5	0.27	0.05	0.26
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	5	0.22	0.07	0.23
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	5	0.22	0.07	0.23
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	5	0.22	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	5	0.22	0.11	0.17
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	5	0.22	0.08	0.22
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	5	0.2	0.07	0.17
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	5	0.2	0.07	0.17
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	5	0.2	0.03	0.2
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	5	0.2	0.03	0.2
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	5	0.2	0.14	0.13
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	5	0.2	0.14	0.13
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	5	0.2	0.14	0.13
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	5	0.17	0.05	0.16
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	5	0.17	0.05	0.16
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	5	0.16	0.04	0.13
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	5	0.16	0.04	0.13
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	5	0.16	0.04	0.13
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	5	0.15	0.04	0.13
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	5	0.15	0.05	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	5	0.15	0.05	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	5	0.15	0.05	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	5	0.15	0.05	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	5	0.15	0.05	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	5	0.15	0.05	0.14
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	5	0.15	0.03	0.13
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	5	0.15	0.02	0.15
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	5	0.14	0.01	0.13
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	5	0.14	0.02	0.13
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	5	0.14	0.02	0.13
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	5	0.14	0.01	0.14
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	5	0.14	0.01	0.14
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	5	0.14	0.01	0.14
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	5	0.13	0.01	0.13
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD11	4	0.7	0.19	0.77
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD12	4	0.7	0.19	0.77
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD13	4	0.7	0.19	0.77
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB1	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB2	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB3	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB1	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB2	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB3	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB1	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB2	4	0.68	0.56	0.61
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB3	4	0.68	0.56	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1633)	1:14:A:GLN:H	1:111:A:ARG:HD3	4	0.65	0.51	0.62
(1,2980)	1:14:A:GLN:HE22	1:109:A:VAL:H	4	0.46	0.24	0.45
(1,3120)	1:72:A:GLN:HE21	1:115:A:GLN:HA	4	0.43	0.5	0.16
(1,2697)	1:112:A:GLN:HG3	1:114:A:LEU:H	4	0.41	0.14	0.41
(1,235)	1:21:A:LEU:HA	1:22:A:ARG:HB3	4	0.38	0.44	0.14
(1,2572)	1:99:A:LYS:H	1:99:A:LYS:HG3	4	0.38	0.06	0.38
(1,2717)	1:116:A:LYS:H	1:116:A:LYS:HB3	4	0.28	0.14	0.24
(1,3128)	1:85:A:MET:HE1	1:92:A:GLN:HE22	4	0.27	0.25	0.14
(1,3128)	1:85:A:MET:HE2	1:92:A:GLN:HE22	4	0.27	0.25	0.14
(1,3128)	1:85:A:MET:HE3	1:92:A:GLN:HE22	4	0.27	0.25	0.14
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG21	4	0.26	0.09	0.24
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG22	4	0.26	0.09	0.24
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG23	4	0.26	0.09	0.24
(1,2852)	1:56:A:TYR:HD1	1:75:A:ASP:H	4	0.25	0.07	0.26
(1,2852)	1:56:A:TYR:HD2	1:75:A:ASP:H	4	0.25	0.07	0.26
(1,2987)	1:4:A:ILE:H	1:8:A:PRO:HD3	4	0.2	0.04	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG21	4	0.2	0.02	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG22	4	0.2	0.02	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG23	4	0.2	0.02	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG21	4	0.2	0.02	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG22	4	0.2	0.02	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG23	4	0.2	0.02	0.2
(1,2111)	1:51:A:THR:H	1:52:A:ASP:HB3	4	0.2	0.05	0.21
(1,2576)	1:98:A:THR:HA	1:100:A:ARG:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD11	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD12	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD13	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD21	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD22	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,2566)	1:97:A:LEU:HD23	1:99:A:LYS:H	4	0.19	0.05	0.2
(1,424)	1:40:A:ASP:HB2	1:41:A:PRO:HD2	4	0.19	0.04	0.18
(1,1662)	1:113:A:SER:HB2	1:114:A:LEU:H	4	0.18	0.03	0.18
(1,1662)	1:113:A:SER:HB3	1:114:A:LEU:H	4	0.18	0.03	0.18
(1,1884)	1:29:A:LEU:HG	1:31:A:PHE:H	4	0.16	0.06	0.14
(1,2411)	1:84:A:ASP:H	1:84:A:ASP:HB2	4	0.16	0.05	0.16
(1,3019)	1:19:A:HIS:HB2	1:105:A:VAL:H	4	0.16	0.04	0.16
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD2	4	0.15	0.05	0.15
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD3	4	0.15	0.05	0.15
(1,981)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	4	0.15	0.04	0.14
(1,981)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	4	0.15	0.04	0.14
(1,981)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	4	0.15	0.04	0.14
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE2	4	0.15	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE3	4	0.15	0.05	0.12
(1,3138)	1:14:A:GLN:H	1:111:A:ARG:HD2	4	0.15	0.02	0.15
(1,2043)	1:41:A:PRO:HA	1:44:A:ASN:H	4	0.15	0.03	0.16
(1,3103)	1:89:A:THR:H	1:92:A:GLN:HA	4	0.13	0.02	0.13
(1,2762)	1:82:A:GLY:H	1:106:A:ARG:H	4	0.13	0.02	0.13
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB2	4	0.12	0.01	0.12
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB3	4	0.12	0.01	0.12
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD11	4	0.11	0.01	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD12	4	0.11	0.01	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD13	4	0.11	0.01	0.11
(1,1929)	1:35:A:GLY:H	1:90:A:HIS:HE1	4	0.11	0.0	0.11
(1,1609)	1:17:A:GLU:HG3	1:19:A:HIS:HD2	4	0.1	0.0	0.1
(1,1669)	1:35:A:GLY:HA3	1:55:A:ILE:H	3	1.54	0.11	1.46
(1,1428)	1:13:A:VAL:HG21	1:110:A:THR:HB	3	1.42	0.1	1.4
(1,1428)	1:13:A:VAL:HG22	1:110:A:THR:HB	3	1.42	0.1	1.4
(1,1428)	1:13:A:VAL:HG23	1:110:A:THR:HB	3	1.42	0.1	1.4
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD2	3	1.26	0.02	1.27
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD3	3	1.26	0.02	1.27
(1,658)	1:61:A:SER:HA	1:62:A:GLU:HB2	3	0.88	0.55	1.2
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	3	0.86	1.03	0.17
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	3	0.86	1.03	0.17
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	3	0.86	1.03	0.17
(1,3066)	1:52:A:ASP:HB3	1:54:A:GLY:HA3	3	0.83	0.39	1.02
(1,142)	1:13:A:VAL:HG11	1:14:A:GLN:HA	3	0.67	0.09	0.67
(1,142)	1:13:A:VAL:HG12	1:14:A:GLN:HA	3	0.67	0.09	0.67
(1,142)	1:13:A:VAL:HG13	1:14:A:GLN:HA	3	0.67	0.09	0.67
(1,141)	1:13:A:VAL:HG11	1:14:A:GLN:H	3	0.49	0.08	0.5
(1,141)	1:13:A:VAL:HG12	1:14:A:GLN:H	3	0.49	0.08	0.5
(1,141)	1:13:A:VAL:HG13	1:14:A:GLN:H	3	0.49	0.08	0.5
(1,2311)	1:72:A:GLN:H	1:72:A:GLN:HE22	3	0.41	0.21	0.43
(1,1738)	1:13:A:VAL:HG11	1:14:A:GLN:H	3	0.38	0.08	0.39
(1,1738)	1:13:A:VAL:HG12	1:14:A:GLN:H	3	0.38	0.08	0.39
(1,1738)	1:13:A:VAL:HG13	1:14:A:GLN:H	3	0.38	0.08	0.39
(1,2912)	1:83:A:TRP:HE1	1:96:A:ARG:HB2	3	0.35	0.17	0.47
(1,2955)	1:13:A:VAL:HG21	1:111:A:ARG:H	3	0.31	0.15	0.25
(1,2955)	1:13:A:VAL:HG22	1:111:A:ARG:H	3	0.31	0.15	0.25
(1,2955)	1:13:A:VAL:HG23	1:111:A:ARG:H	3	0.31	0.15	0.25
(1,3093)	1:24:A:GLY:HA2	1:25:A:GLU:HG3	3	0.31	0.13	0.33
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD11	3	0.3	0.07	0.34
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD12	3	0.3	0.07	0.34
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD13	3	0.3	0.07	0.34
(1,2012)	1:40:A:ASP:H	1:41:A:PRO:HD2	3	0.3	0.06	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2986)	1:72:A:GLN:HE22	1:113:A:SER:H	3	0.29	0.19	0.19
(1,2721)	1:116:A:LYS:HA	1:117:A:ALA:H	3	0.27	0.09	0.29
(1,55)	1:4:A:ILE:HB	1:5:A:PRO:HD3	3	0.26	0.12	0.18
(1,1375)	1:3:A:TYR:HE1	1:5:A:PRO:HD2	3	0.26	0.03	0.26
(1,1375)	1:3:A:TYR:HE2	1:5:A:PRO:HD2	3	0.26	0.03	0.26
(1,843)	1:95:A:LYS:HA	1:95:A:LYS:HG2	3	0.24	0.0	0.24
(1,2903)	1:79:A:GLN:HB2	1:83:A:TRP:H	3	0.23	0.16	0.13
(1,3156)	1:36:A:GLY:H	1:55:A:ILE:H	3	0.2	0.07	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	3	0.19	0.04	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	3	0.19	0.04	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	3	0.19	0.04	0.19
(1,1459)	1:48:A:GLU:HB3	1:49:A:ASP:HB3	3	0.18	0.05	0.17
(1,411)	1:39:A:GLN:HG2	1:90:A:HIS:HB3	3	0.18	0.04	0.19
(1,1458)	1:23:A:GLN:HB2	1:26:A:ASN:HB2	3	0.18	0.02	0.18
(1,14)	1:15:A:ARG:HD2	1:16:A:VAL:HA	3	0.17	0.05	0.17
(1,14)	1:15:A:ARG:HD3	1:16:A:VAL:HA	3	0.17	0.05	0.17
(1,1408)	1:34:A:GLY:HA3	1:90:A:HIS:HE1	3	0.16	0.03	0.15
(1,1536)	1:13:A:VAL:HA	1:110:A:THR:HA	3	0.16	0.04	0.15
(1,2564)	1:95:A:LYS:HE2	1:99:A:LYS:H	3	0.16	0.01	0.16
(1,2564)	1:95:A:LYS:HE3	1:99:A:LYS:H	3	0.16	0.01	0.16
(1,2176)	1:32:A:SER:HB2	1:59:A:ARG:H	3	0.15	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,850)	1:95:A:LYS:HE2	1:99:A:LYS:HB3	3	0.15	0.03	0.16
(1,850)	1:95:A:LYS:HE3	1:99:A:LYS:HB3	3	0.15	0.03	0.16
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG2	3	0.14	0.01	0.14
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG3	3	0.14	0.01	0.14
(1,551)	1:52:A:ASP:HA	1:53:A:LYS:H	3	0.14	0.03	0.13
(1,2452)	1:36:A:GLY:HA2	1:90:A:HIS:H	3	0.14	0.03	0.15
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD2	3	0.14	0.02	0.13
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD3	3	0.14	0.02	0.13
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG11	3	0.14	0.03	0.13
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG12	3	0.14	0.03	0.13
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG13	3	0.14	0.03	0.13
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD11	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD12	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD13	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD11	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD12	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD13	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD11	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD12	3	0.13	0.02	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD13	3	0.13	0.02	0.14
(1,1667)	1:14:A:GLN:HA	1:14:A:GLN:HE22	3	0.13	0.01	0.12
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD2	3	0.13	0.02	0.13
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD3	3	0.13	0.02	0.13
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD21	3	0.13	0.02	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD22	3	0.13	0.02	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD23	3	0.13	0.02	0.14
(1,2981)	1:50:A:LYS:HD2	1:110:A:THR:H	3	0.13	0.03	0.11
(1,2981)	1:50:A:LYS:HD3	1:110:A:THR:H	3	0.13	0.03	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG21	3	0.13	0.03	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG22	3	0.13	0.03	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG23	3	0.13	0.03	0.11
(1,2538)	1:95:A:LYS:H	1:95:A:LYS:HB2	3	0.12	0.0	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD11	3	0.12	0.01	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD12	3	0.12	0.01	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD13	3	0.12	0.01	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD21	3	0.12	0.01	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD22	3	0.12	0.01	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD23	3	0.12	0.01	0.12
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE1	3	0.12	0.01	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE2	3	0.12	0.01	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE3	3	0.12	0.01	0.13
(2,15)	1:92:A:GLN:O	1:96:A:ARG:H	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2559)	1:97:A:LEU:HG	1:98:A:THR:H	3	0.12	0.01	0.11
(1,2974)	1:97:A:LEU:H	1:97:A:LEU:HG	3	0.12	0.01	0.11
(1,3015)	1:89:A:THR:HG21	1:92:A:GLN:HE22	3	0.12	0.01	0.12
(1,3015)	1:89:A:THR:HG22	1:92:A:GLN:HE22	3	0.12	0.01	0.12
(1,3015)	1:89:A:THR:HG23	1:92:A:GLN:HE22	3	0.12	0.01	0.12
(1,217)	1:18:A:ILE:HD11	1:19:A:HIS:H	3	0.11	0.01	0.11
(1,217)	1:18:A:ILE:HD12	1:19:A:HIS:H	3	0.11	0.01	0.11
(1,217)	1:18:A:ILE:HD13	1:19:A:HIS:H	3	0.11	0.01	0.11
(1,1426)	1:13:A:VAL:HG21	1:14:A:GLN:H	3	0.11	0.01	0.11
(1,1426)	1:13:A:VAL:HG22	1:14:A:GLN:H	3	0.11	0.01	0.11
(1,1426)	1:13:A:VAL:HG23	1:14:A:GLN:H	3	0.11	0.01	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG21	3	0.11	0.01	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG22	3	0.11	0.01	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG23	3	0.11	0.01	0.11
(1,2917)	1:80:A:VAL:HG11	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,2917)	1:80:A:VAL:HG12	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,2917)	1:80:A:VAL:HG13	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,2917)	1:80:A:VAL:HG21	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,2917)	1:80:A:VAL:HG22	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,2917)	1:80:A:VAL:HG23	1:84:A:ASP:H	3	0.11	0.0	0.11
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE2	3	0.11	0.01	0.1
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE3	3	0.11	0.01	0.1
(1,2314)	1:71:A:LEU:HA	1:72:A:GLN:HE22	3	0.1	0.0	0.1
(1,644)	1:60:A:VAL:HG11	1:67:A:GLU:HB3	2	1.88	0.16	1.88
(1,644)	1:60:A:VAL:HG12	1:67:A:GLU:HB3	2	1.88	0.16	1.88
(1,644)	1:60:A:VAL:HG13	1:67:A:GLU:HB3	2	1.88	0.16	1.88
(1,3004)	1:16:A:VAL:HG11	1:66:A:ALA:H	2	1.68	0.13	1.68
(1,3004)	1:16:A:VAL:HG12	1:66:A:ALA:H	2	1.68	0.13	1.68
(1,3004)	1:16:A:VAL:HG13	1:66:A:ALA:H	2	1.68	0.13	1.68
(1,2223)	1:60:A:VAL:HG11	1:64:A:GLY:H	2	1.56	0.09	1.56
(1,2223)	1:60:A:VAL:HG12	1:64:A:GLY:H	2	1.56	0.09	1.56
(1,2223)	1:60:A:VAL:HG13	1:64:A:GLY:H	2	1.56	0.09	1.56
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	2	1.31	0.01	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	2	1.31	0.01	1.31
(1,2937)	1:16:A:VAL:HG11	1:107:A:LEU:H	2	1.29	0.02	1.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2937)	1:16:A:VAL:HG12	1:107:A:LEU:H	2	1.29	0.02	1.29
(1,2937)	1:16:A:VAL:HG13	1:107:A:LEU:H	2	1.29	0.02	1.29
(1,2212)	1:60:A:VAL:HG11	1:63:A:GLY:H	2	1.27	0.11	1.27
(1,2212)	1:60:A:VAL:HG12	1:63:A:GLY:H	2	1.27	0.11	1.27
(1,2212)	1:60:A:VAL:HG13	1:63:A:GLY:H	2	1.27	0.11	1.27
(1,193)	1:16:A:VAL:HG11	1:17:A:GLU:HA	2	1.26	0.01	1.26
(1,193)	1:16:A:VAL:HG12	1:17:A:GLU:HA	2	1.26	0.01	1.26
(1,193)	1:16:A:VAL:HG13	1:17:A:GLU:HA	2	1.26	0.01	1.26
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG21	2	1.09	0.09	1.09
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG22	2	1.09	0.09	1.09
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG23	2	1.09	0.09	1.09
(1,2518)	1:88:A:VAL:HG11	1:94:A:ARG:H	2	1.09	0.96	1.09
(1,2518)	1:88:A:VAL:HG12	1:94:A:ARG:H	2	1.09	0.96	1.09
(1,2518)	1:88:A:VAL:HG13	1:94:A:ARG:H	2	1.09	0.96	1.09
(1,2244)	1:60:A:VAL:HG11	1:67:A:GLU:H	2	1.02	0.07	1.02
(1,2244)	1:60:A:VAL:HG12	1:67:A:GLU:H	2	1.02	0.07	1.02
(1,2244)	1:60:A:VAL:HG13	1:67:A:GLU:H	2	1.02	0.07	1.02
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG21	2	0.92	0.05	0.92
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG22	2	0.92	0.05	0.92
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG23	2	0.92	0.05	0.92
(1,683)	1:62:A:GLU:HB3	1:63:A:GLY:HA3	2	0.83	0.03	0.83
(1,1485)	1:60:A:VAL:HG21	1:73:A:ILE:HA	2	0.76	0.02	0.76
(1,1485)	1:60:A:VAL:HG22	1:73:A:ILE:HA	2	0.76	0.02	0.76
(1,1485)	1:60:A:VAL:HG23	1:73:A:ILE:HA	2	0.76	0.02	0.76
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB2	2	0.64	0.08	0.64
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB3	2	0.64	0.08	0.64
(1,2466)	1:90:A:HIS:H	1:91:A:ASP:HB2	2	0.6	0.04	0.6
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	2	0.54	0.01	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	2	0.54	0.01	0.54
(1,2533)	1:91:A:ASP:HB3	1:95:A:LYS:H	2	0.48	0.02	0.48
(1,1437)	1:16:A:VAL:HG11	1:107:A:LEU:H	2	0.47	0.02	0.47
(1,1437)	1:16:A:VAL:HG12	1:107:A:LEU:H	2	0.47	0.02	0.47
(1,1437)	1:16:A:VAL:HG13	1:107:A:LEU:H	2	0.47	0.02	0.47
(1,2958)	1:72:A:GLN:HE22	1:111:A:ARG:H	2	0.44	0.29	0.44
(1,2689)	1:111:A:ARG:HG3	1:113:A:SER:H	2	0.4	0.21	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2909)	1:81:A:ASN:HB3	1:83:A:TRP:HE1	2	0.34	0.0	0.34
(1,2129)	1:53:A:LYS:H	1:54:A:GLY:HA3	2	0.33	0.05	0.33
(1,2220)	1:62:A:GLU:HB3	1:63:A:GLY:H	2	0.32	0.01	0.32
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG2	2	0.3	0.01	0.3
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG3	2	0.3	0.01	0.3
(1,153)	1:14:A:GLN:H	1:14:A:GLN:HG3	2	0.26	0.02	0.26
(1,1992)	1:39:A:GLN:HA	1:39:A:GLN:HE22	2	0.25	0.11	0.25
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG21	2	0.24	0.01	0.24
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG22	2	0.24	0.01	0.24
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG23	2	0.24	0.01	0.24
(1,753)	1:60:A:VAL:HG11	1:67:A:GLU:HA	2	0.24	0.01	0.24
(1,753)	1:60:A:VAL:HG12	1:67:A:GLU:HA	2	0.24	0.01	0.24
(1,753)	1:60:A:VAL:HG13	1:67:A:GLU:HA	2	0.24	0.01	0.24
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB2	2	0.24	0.03	0.24
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB3	2	0.24	0.03	0.24
(1,670)	1:60:A:VAL:HG11	1:62:A:GLU:HA	2	0.22	0.1	0.22
(1,670)	1:60:A:VAL:HG12	1:62:A:GLU:HA	2	0.22	0.1	0.22
(1,670)	1:60:A:VAL:HG13	1:62:A:GLU:HA	2	0.22	0.1	0.22
(1,760)	1:60:A:VAL:HG11	1:67:A:GLU:HG2	2	0.22	0.07	0.22
(1,760)	1:60:A:VAL:HG12	1:67:A:GLU:HG2	2	0.22	0.07	0.22
(1,760)	1:60:A:VAL:HG13	1:67:A:GLU:HG2	2	0.22	0.07	0.22
(1,1476)	1:58:A:THR:HG21	1:59:A:ARG:HG2	2	0.22	0.08	0.22
(1,1476)	1:58:A:THR:HG22	1:59:A:ARG:HG2	2	0.22	0.08	0.22
(1,1476)	1:58:A:THR:HG23	1:59:A:ARG:HG2	2	0.22	0.08	0.22
(1,3021)	1:115:A:GLN:HG2	1:117:A:ALA:H	2	0.21	0.09	0.21
(1,3021)	1:115:A:GLN:HG3	1:117:A:ALA:H	2	0.21	0.09	0.21
(1,3037)	1:35:A:GLY:H	1:39:A:GLN:HG3	2	0.2	0.06	0.2
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD11	2	0.2	0.09	0.2
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD12	2	0.2	0.09	0.2
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD13	2	0.2	0.09	0.2
(1,2039)	1:43:A:GLN:HB3	1:43:A:GLN:HE21	2	0.19	0.0	0.19
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB2	2	0.19	0.01	0.19
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB3	2	0.19	0.01	0.19
(1,359)	1:36:A:GLY:HA3	1:37:A:ILE:HG13	2	0.18	0.02	0.18
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD11	2	0.17	0.0	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD12	2	0.17	0.0	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD13	2	0.17	0.0	0.17
(1,2578)	1:99:A:LYS:HG2	1:100:A:ARG:H	2	0.17	0.03	0.17
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD21	2	0.17	0.03	0.17
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD22	2	0.17	0.03	0.17
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD23	2	0.17	0.03	0.17
(1,1677)	1:35:A:GLY:HA3	1:56:A:TYR:H	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,87)	1:8:A:PRO:HA	1:9:A:VAL:H	2	0.16	0.02	0.16
(1,1418)	1:7:A:GLN:HG2	1:8:A:PRO:HD3	2	0.16	0.01	0.16
(1,1418)	1:7:A:GLN:HG3	1:8:A:PRO:HD3	2	0.16	0.01	0.16
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG2	2	0.16	0.01	0.16
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG3	2	0.16	0.01	0.16
(1,2098)	1:49:A:ASP:HB3	1:50:A:LYS:H	2	0.16	0.0	0.16
(1,1757)	1:15:A:ARG:H	1:15:A:ARG:HB3	2	0.16	0.02	0.16
(1,2736)	1:119:A:GLN:H	1:119:A:GLN:HB3	2	0.15	0.01	0.15
(1,3064)	1:52:A:ASP:HA	1:54:A:GLY:H	2	0.15	0.01	0.15
(1,548)	1:51:A:THR:H	1:51:A:THR:HG21	2	0.15	0.03	0.15
(1,548)	1:51:A:THR:H	1:51:A:THR:HG22	2	0.15	0.03	0.15
(1,548)	1:51:A:THR:H	1:51:A:THR:HG23	2	0.15	0.03	0.15
(1,1295)	1:91:A:ASP:H	1:91:A:ASP:HB2	2	0.15	0.03	0.15
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG21	2	0.15	0.03	0.15
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG22	2	0.15	0.03	0.15
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG23	2	0.15	0.03	0.15
(1,2670)	1:112:A:GLN:H	1:112:A:GLN:HB2	2	0.15	0.03	0.15
(1,2816)	1:23:A:GLN:HB2	1:26:A:ASN:HD21	2	0.15	0.02	0.15
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD2	2	0.15	0.03	0.15
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD3	2	0.15	0.03	0.15
(1,1624)	1:46:A:PHE:H	1:47:A:SER:HB2	2	0.14	0.03	0.14
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG2	2	0.14	0.03	0.14
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG3	2	0.14	0.03	0.14
(1,1857)	1:27:A:LEU:H	1:27:A:LEU:HG	2	0.14	0.03	0.14
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE1	2	0.14	0.03	0.14
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE2	2	0.14	0.03	0.14
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD2	2	0.14	0.01	0.14
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD3	2	0.14	0.01	0.14
(1,475)	1:44:A:ASN:H	1:45:A:PRO:HD2	2	0.13	0.02	0.13
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG21	2	0.13	0.01	0.13
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG22	2	0.13	0.01	0.13
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG23	2	0.13	0.01	0.13
(1,2052)	1:44:A:ASN:H	1:45:A:PRO:HD2	2	0.13	0.02	0.13
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD2	2	0.13	0.02	0.13
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD3	2	0.13	0.02	0.13
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG21	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG22	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG23	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG21	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG22	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG23	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG21	2	0.12	0.02	0.12

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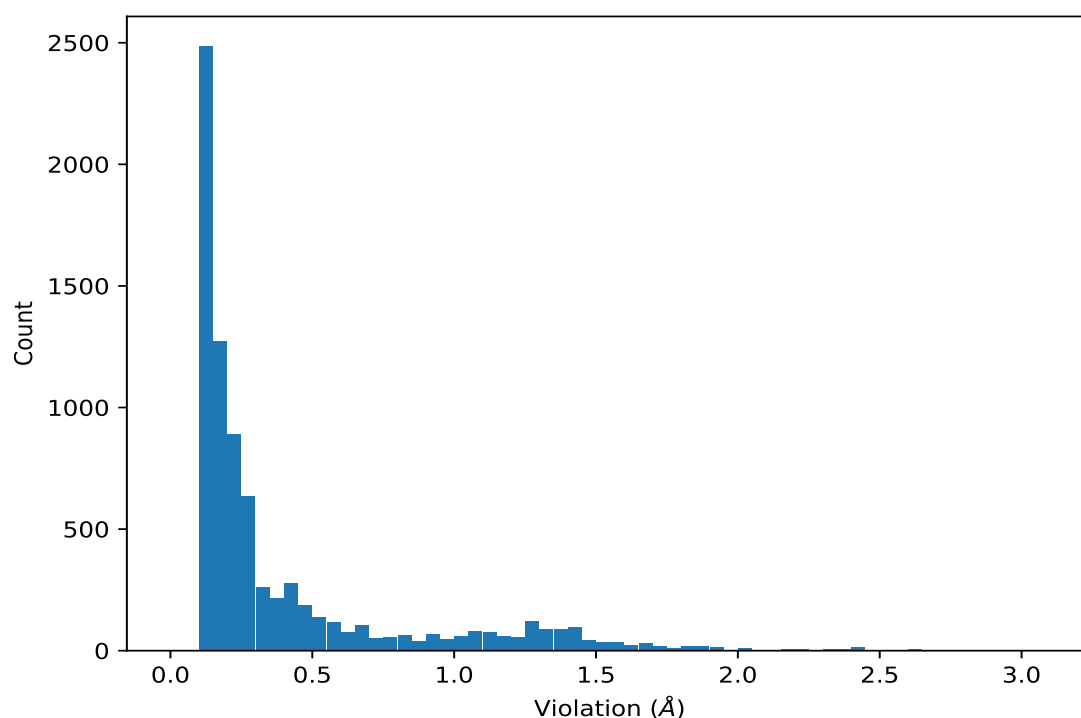
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG22	2	0.12	0.02	0.12
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG23	2	0.12	0.02	0.12
(1,2370)	1:79:A:GLN:HA	1:79:A:GLN:HE22	2	0.12	0.02	0.12
(1,2800)	1:20:A:LYS:HE2	1:22:A:ARG:H	2	0.12	0.01	0.12
(1,2800)	1:20:A:LYS:HE3	1:22:A:ARG:H	2	0.12	0.01	0.12
(1,1309)	1:88:A:VAL:HA	1:92:A:GLN:HB2	2	0.12	0.02	0.12
(1,320)	1:32:A:SER:HB2	1:59:A:ARG:HA	2	0.12	0.01	0.12
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG21	2	0.12	0.01	0.12
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG22	2	0.12	0.01	0.12
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG23	2	0.12	0.01	0.12
(1,1350)	1:33:A:ILE:HD11	1:94:A:ARG:HB3	2	0.12	0.0	0.12
(1,1350)	1:33:A:ILE:HD12	1:94:A:ARG:HB3	2	0.12	0.0	0.12
(1,1350)	1:33:A:ILE:HD13	1:94:A:ARG:HB3	2	0.12	0.0	0.12
(1,1404)	1:33:A:ILE:HD11	1:90:A:HIS:HE1	2	0.12	0.02	0.12
(1,1404)	1:33:A:ILE:HD12	1:90:A:HIS:HE1	2	0.12	0.02	0.12
(1,1404)	1:33:A:ILE:HD13	1:90:A:HIS:HE1	2	0.12	0.02	0.12
(1,128)	1:11:A:ALA:HB1	1:12:A:VAL:HA	2	0.12	0.0	0.12
(1,128)	1:11:A:ALA:HB2	1:12:A:VAL:HA	2	0.12	0.0	0.12
(1,128)	1:11:A:ALA:HB3	1:12:A:VAL:HA	2	0.12	0.0	0.12
(1,319)	1:32:A:SER:HB2	1:59:A:ARG:H	2	0.12	0.0	0.12
(1,1076)	1:116:A:LYS:HB2	1:117:A:ALA:H	2	0.12	0.0	0.12
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD2	2	0.11	0.0	0.11
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD3	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD11	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD12	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD13	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD21	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD22	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,887)	1:97:A:LEU:HD23	1:98:A:THR:HA	2	0.11	0.0	0.11
(1,1928)	1:35:A:GLY:H	1:90:A:HIS:HD2	2	0.11	0.0	0.11
(1,1985)	1:39:A:GLN:HE22	1:91:A:ASP:H	2	0.11	0.0	0.11
(2,17)	1:94:A:ARG:O	1:98:A:THR:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:32:A:SER:H	1:58:A:THR:O	2	3.08
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	17	2.77
(2,59)	1:32:A:SER:N	1:58:A:THR:O	2	2.75
(2,53)	1:32:A:SER:H	1:58:A:THR:O	6	2.75
(2,53)	1:32:A:SER:H	1:58:A:THR:O	9	2.7
(2,53)	1:32:A:SER:H	1:58:A:THR:O	17	2.7
(2,53)	1:32:A:SER:H	1:58:A:THR:O	4	2.69
(2,53)	1:32:A:SER:H	1:58:A:THR:O	15	2.69
(2,53)	1:32:A:SER:H	1:58:A:THR:O	8	2.68
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	12	2.68
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	14	2.65
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	14	2.65
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	14	2.65
(2,53)	1:32:A:SER:H	1:58:A:THR:O	1	2.63
(2,53)	1:32:A:SER:H	1:58:A:THR:O	3	2.62
(2,53)	1:32:A:SER:H	1:58:A:THR:O	13	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:32:A:SER:H	1:58:A:THR:O	7	2.46
(2,59)	1:32:A:SER:N	1:58:A:THR:O	6	2.44
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	14	2.44
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	14	2.44
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	14	2.44
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	17	2.43
(2,59)	1:32:A:SER:N	1:58:A:THR:O	17	2.42
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	20	2.42
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	20	2.42
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	20	2.42
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	20	2.42
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	20	2.42
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	20	2.42
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	20	2.42
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	20	2.42
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	20	2.42
(2,59)	1:32:A:SER:N	1:58:A:THR:O	4	2.39
(2,59)	1:32:A:SER:N	1:58:A:THR:O	9	2.39
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	12	2.39
(2,59)	1:32:A:SER:N	1:58:A:THR:O	8	2.38
(2,59)	1:32:A:SER:N	1:58:A:THR:O	15	2.37
(2,59)	1:32:A:SER:N	1:58:A:THR:O	3	2.35
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	12	2.34
(2,59)	1:32:A:SER:N	1:58:A:THR:O	1	2.33
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	14	2.31
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	14	2.31
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	14	2.31
(2,59)	1:32:A:SER:N	1:58:A:THR:O	13	2.27
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	12	2.23
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	12	2.23
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	12	2.23
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	12	2.21
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	7	2.2
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	12	2.19
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	19	2.19
(2,59)	1:32:A:SER:N	1:58:A:THR:O	7	2.18
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	7	2.16
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	7	2.16
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	7	2.16
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	5	2.15
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	12	2.1
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	12	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	12	2.1
(1,3136)	1:88:A:VAL:HG11	1:91:A:ASP:H	13	2.09
(1,3136)	1:88:A:VAL:HG12	1:91:A:ASP:H	13	2.09
(1,3136)	1:88:A:VAL:HG13	1:91:A:ASP:H	13	2.09
(1,2518)	1:88:A:VAL:HG11	1:94:A:ARG:H	13	2.05
(1,2518)	1:88:A:VAL:HG12	1:94:A:ARG:H	13	2.05
(1,2518)	1:88:A:VAL:HG13	1:94:A:ARG:H	13	2.05
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	5	2.04
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	5	2.04
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	5	2.04
(1,644)	1:60:A:VAL:HG11	1:67:A:GLU:HB3	12	2.04
(1,644)	1:60:A:VAL:HG12	1:67:A:GLU:HB3	12	2.04
(1,644)	1:60:A:VAL:HG13	1:67:A:GLU:HB3	12	2.04
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	14	2.0
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	14	2.0
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	14	2.0
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	17	1.96
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	19	1.95
(1,2349)	1:77:A:ILE:H	1:78:A:MET:HE1	20	1.94
(1,2349)	1:77:A:ILE:H	1:78:A:MET:HE2	20	1.94
(1,2349)	1:77:A:ILE:H	1:78:A:MET:HE3	20	1.94
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	11	1.93
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	11	1.93
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	11	1.93
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	4	1.93
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	2	1.93
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	2	1.93
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	2	1.93
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	16	1.92
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	16	1.92
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	16	1.92
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	5	1.9
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	5	1.9
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	5	1.9
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	19	1.89
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	19	1.89
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	19	1.89
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	19	1.89
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	19	1.89
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	13	1.89
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	19	1.88
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	19	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	19	1.88
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	11	1.88
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	12	1.87
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	19	1.86
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	3	1.86
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	5	1.85
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	12	1.83
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	12	1.83
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	12	1.83
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	12	1.83
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	5	1.82
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	5	1.81
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	20	1.81
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	20	1.81
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	20	1.81
(1,3004)	1:16:A:VAL:HG11	1:66:A:ALA:H	6	1.81
(1,3004)	1:16:A:VAL:HG12	1:66:A:ALA:H	6	1.81
(1,3004)	1:16:A:VAL:HG13	1:66:A:ALA:H	6	1.81
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	11	1.81
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	12	1.8
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	19	1.8
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	14	1.8
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	14	1.8
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	14	1.8
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	11	1.79
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	11	1.79
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	11	1.79
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	8	1.78
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	9	1.78
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	3	1.77
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	3	1.77
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	3	1.77
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	18	1.76
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	18	1.76
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	18	1.76
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	5	1.76
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	11	1.74
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	11	1.74
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	11	1.74
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	4	1.74
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	9	1.74
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	6	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	8	1.73
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	18	1.73
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	2	1.72
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	8	1.72
(1,644)	1:60:A:VAL:HG11	1:67:A:GLU:HB3	7	1.72
(1,644)	1:60:A:VAL:HG12	1:67:A:GLU:HB3	7	1.72
(1,644)	1:60:A:VAL:HG13	1:67:A:GLU:HB3	7	1.72
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	9	1.72
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	3	1.71
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	4	1.71
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	2	1.71
(1,1669)	1:35:A:GLY:HA3	1:55:A:ILE:H	12	1.7
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	17	1.7
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	19	1.69
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	2	1.69
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	3	1.69
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	18	1.69
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	11	1.68
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	20	1.68
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	8	1.68
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	19	1.67
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	10	1.67
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	10	1.67
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	10	1.67
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	17	1.67
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	19	1.67
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	3	1.67
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	18	1.67
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	17	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	4	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	4	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	4	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	18	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	18	1.66
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	18	1.66
(1,2223)	1:60:A:VAL:HG11	1:64:A:GLY:H	12	1.66
(1,2223)	1:60:A:VAL:HG12	1:64:A:GLY:H	12	1.66
(1,2223)	1:60:A:VAL:HG13	1:64:A:GLY:H	12	1.66
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	8	1.66
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	5	1.66
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	9	1.65
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	11	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	16	1.65
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	16	1.65
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	16	1.65
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	12	1.64
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	9	1.64
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	17	1.64
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	20	1.64
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	20	1.64
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	20	1.64
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	5	1.64
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	12	1.63
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	12	1.63
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	12	1.63
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	12	1.63
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	2	1.62
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	12	1.62
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	1	1.61
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	15	1.61
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	8	1.61
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	13	1.61
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	6	1.6
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	6	1.6
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	1	1.59
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	20	1.59
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	15	1.58
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	11	1.58
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	2	1.58
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	14	1.58
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	13	1.57
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	18	1.57
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	15	1.57
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	16	1.57
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	13	1.56
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	19	1.56
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	5	1.56
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	5	1.56
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	5	1.56
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	8	1.55
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	11	1.55
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	2	1.55
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	2	1.55
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	2	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	2	1.55
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	2	1.55
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	2	1.55
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	2	1.55
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	2	1.55
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	2	1.55
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	16	1.55
(1,3004)	1:16:A:VAL:HG11	1:66:A:ALA:H	17	1.55
(1,3004)	1:16:A:VAL:HG12	1:66:A:ALA:H	17	1.55
(1,3004)	1:16:A:VAL:HG13	1:66:A:ALA:H	17	1.55
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	10	1.55
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	2	1.55
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	11	1.55
(1,1428)	1:13:A:VAL:HG21	1:110:A:THR:HB	5	1.55
(1,1428)	1:13:A:VAL:HG22	1:110:A:THR:HB	5	1.55
(1,1428)	1:13:A:VAL:HG23	1:110:A:THR:HB	5	1.55
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	16	1.55
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	19	1.54
(1,2904)	1:79:A:GLN:HG3	1:83:A:TRP:H	13	1.54
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	8	1.54
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	9	1.54
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	19	1.54
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	15	1.54
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	16	1.54
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	7	1.53
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	16	1.53
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	8	1.53
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	4	1.53
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	6	1.53
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	11	1.53
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	13	1.53
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	13	1.53
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	13	1.53
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	18	1.53
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	9	1.52
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	2	1.52
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	4	1.52
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	19	1.51
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	19	1.51
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	19	1.51
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	3	1.51
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	9	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	16	1.51
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	2	1.51
(2,53)	1:32:A:SER:H	1:58:A:THR:O	19	1.5
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	1	1.5
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	4	1.5
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	10	1.5
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	8	1.5
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	18	1.5
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	7	1.49
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	18	1.49
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	6	1.49
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	11	1.48
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	11	1.48
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	11	1.48
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	11	1.48
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	11	1.48
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	11	1.48
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	11	1.48
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	11	1.48
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	11	1.48
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	17	1.48
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	20	1.48
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	1	1.48
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	19	1.48
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	15	1.48
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	11	1.48
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	19	1.48
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	5	1.47
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	10	1.47
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	10	1.47
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	20	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	15	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	15	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	15	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	20	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	20	1.47
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	20	1.47
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	6	1.47
(1,2223)	1:60:A:VAL:HG11	1:64:A:GLY:H	7	1.47
(1,2223)	1:60:A:VAL:HG12	1:64:A:GLY:H	7	1.47
(1,2223)	1:60:A:VAL:HG13	1:64:A:GLY:H	7	1.47
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	15	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	18	1.47
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	1	1.47
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	2	1.46
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	3	1.46
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	14	1.46
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	6	1.46
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	1	1.46
(1,1669)	1:35:A:GLY:HA3	1:55:A:ILE:H	5	1.46
(1,1669)	1:35:A:GLY:HA3	1:55:A:ILE:H	19	1.46
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	19	1.46
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	3	1.45
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	6	1.45
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	20	1.45
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	20	1.45
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	20	1.45
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	20	1.45
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	20	1.45
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	20	1.45
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	20	1.45
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	20	1.45
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	20	1.45
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	3	1.45
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	3	1.45
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	3	1.45
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	7	1.45
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	7	1.45
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	2	1.45
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	2	1.44
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	5	1.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	11	1.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	11	1.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	11	1.44
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	6	1.44
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	16	1.44
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	19	1.44
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	12	1.44
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	12	1.44
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	12	1.44
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	15	1.44
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	15	1.44
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	10	1.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	4	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	4	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	4	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	7	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	7	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	7	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	9	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	9	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	9	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	13	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	13	1.43
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	13	1.43
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	8	1.43
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	8	1.43
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	8	1.43
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	2	1.43
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	7	1.43
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	11	1.43
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	5	1.43
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	5	1.43
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	6	1.43
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	12	1.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	12	1.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	12	1.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	12	1.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	12	1.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	12	1.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	12	1.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	12	1.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	12	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	14	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	14	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	14	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	18	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	18	1.42
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	18	1.42
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	15	1.42
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	4	1.42
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	15	1.42
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	15	1.42
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	15	1.42
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	12	1.42
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	12	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	12	1.42
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	10	1.42
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	12	1.41
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	4	1.41
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	4	1.41
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	4	1.41
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	4	1.41
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	4	1.41
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	4	1.41
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	4	1.41
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	4	1.41
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	4	1.41
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	6	1.41
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	6	1.41
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	6	1.41
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	1	1.41
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	1	1.41
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	1	1.41
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	13	1.41
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	16	1.41
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	17	1.41
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	12	1.41
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	16	1.4
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	12	1.4
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	9	1.4
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	4	1.4
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	14	1.4
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	1	1.4
(1,1484)	1:60:A:VAL:HG21	1:72:A:GLN:HA	12	1.4
(1,1484)	1:60:A:VAL:HG22	1:72:A:GLN:HA	12	1.4
(1,1484)	1:60:A:VAL:HG23	1:72:A:GLN:HA	12	1.4
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	4	1.4
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	4	1.4
(1,1428)	1:13:A:VAL:HG21	1:110:A:THR:HB	19	1.4
(1,1428)	1:13:A:VAL:HG22	1:110:A:THR:HB	19	1.4
(1,1428)	1:13:A:VAL:HG23	1:110:A:THR:HB	19	1.4
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	14	1.4
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	14	1.4
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	14	1.4
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	17	1.39
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	1	1.39
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	7	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	5	1.39
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	13	1.39
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	13	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	5	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	5	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	5	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	19	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	19	1.39
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	19	1.39
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	12	1.39
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	15	1.38
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	1	1.38
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	20	1.38
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	15	1.38
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	12	1.38
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	12	1.38
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	12	1.38
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	11	1.38
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	1	1.37
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	1	1.37
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	1	1.37
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	9	1.37
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	9	1.37
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	9	1.37
(1,2212)	1:60:A:VAL:HG11	1:63:A:GLY:H	12	1.37
(1,2212)	1:60:A:VAL:HG12	1:63:A:GLY:H	12	1.37
(1,2212)	1:60:A:VAL:HG13	1:63:A:GLY:H	12	1.37
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	9	1.37
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	20	1.37
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	7	1.37
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	5	1.37
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	5	1.37
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	5	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	9	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	9	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	17	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	17	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	19	1.37
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	19	1.37
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	18	1.36
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	17	1.36
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	12	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	14	1.36
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	16	1.36
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB1	6	1.36
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB2	6	1.36
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB3	6	1.36
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB1	6	1.36
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB2	6	1.36
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB3	6	1.36
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB1	6	1.36
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB2	6	1.36
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB3	6	1.36
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	1	1.36
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	12	1.36
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	12	1.36
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	3	1.36
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	3	1.36
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	3	1.36
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	11	1.36
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	13	1.35
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	13	1.35
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	7	1.35
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	11	1.35
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	14	1.35
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	8	1.35
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	8	1.35
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	7	1.35
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	7	1.35
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	7	1.35
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	8	1.34
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	8	1.34
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	8	1.34
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	17	1.34
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	17	1.34
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	17	1.34
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	18	1.34
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	10	1.34
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	20	1.34
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	4	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	1	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	1	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	7	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	7	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	15	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	15	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	18	1.34
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	18	1.34
(1,658)	1:61:A:SER:HA	1:62:A:GLU:HB2	16	1.34
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	15	1.34
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	20	1.34
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	19	1.33
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	19	1.33
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	19	1.33
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	14	1.33
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	14	1.33
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	14	1.33
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	18	1.33
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	18	1.33
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	18	1.33
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	9	1.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	9	1.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	9	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	9	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	9	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	9	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	9	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	9	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	9	1.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	15	1.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	15	1.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	15	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	15	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	15	1.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	15	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	15	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	15	1.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	15	1.32
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	7	1.32
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	16	1.32
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	20	1.32
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	15	1.32
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	20	1.32
(1,2937)	1:16:A:VAL:HG11	1:107:A:LEU:H	17	1.31
(1,2937)	1:16:A:VAL:HG12	1:107:A:LEU:H	17	1.31
(1,2937)	1:16:A:VAL:HG13	1:107:A:LEU:H	17	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	20	1.31
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	12	1.31
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	12	1.31
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	12	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	12	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	12	1.31
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	12	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	12	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	12	1.31
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	12	1.31
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	6	1.3
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	6	1.3
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	6	1.3
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	9	1.3
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	20	1.3
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	10	1.3
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	10	1.3
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	17	1.3
(1,1428)	1:13:A:VAL:HG21	1:110:A:THR:HB	11	1.3
(1,1428)	1:13:A:VAL:HG22	1:110:A:THR:HB	11	1.3
(1,1428)	1:13:A:VAL:HG23	1:110:A:THR:HB	11	1.3
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	7	1.3
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	7	1.3
(1,742)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	7	1.3
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	7	1.3
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	7	1.3
(1,742)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	7	1.3
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	7	1.3
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	7	1.3
(1,742)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	7	1.3
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	1	1.3
(1,3120)	1:72:A:GLN:HE21	1:115:A:GLN:HA	1	1.29
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	14	1.29
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	6	1.29
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	4	1.29
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	7	1.29
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	20	1.29
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	20	1.29
(1,1430)	1:14:A:GLN:HG2	1:109:A:VAL:HG11	14	1.29
(1,1430)	1:14:A:GLN:HG2	1:109:A:VAL:HG12	14	1.29
(1,1430)	1:14:A:GLN:HG2	1:109:A:VAL:HG13	14	1.29
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	13	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	13	1.29
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	13	1.29
(1,3145)	1:105:A:VAL:H	1:106:A:ARG:HG2	5	1.28
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	3	1.28
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	3	1.28
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	3	1.28
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	5	1.28
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	17	1.28
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	1	1.28
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	8	1.28
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	15	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	15	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	15	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	15	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	20	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	20	1.28
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	20	1.28
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	3	1.28
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	3	1.28
(1,1335)	1:88:A:VAL:HG11	1:93:A:ALA:HB1	13	1.28
(1,1335)	1:88:A:VAL:HG11	1:93:A:ALA:HB2	13	1.28
(1,1335)	1:88:A:VAL:HG11	1:93:A:ALA:HB3	13	1.28
(1,1335)	1:88:A:VAL:HG12	1:93:A:ALA:HB1	13	1.28
(1,1335)	1:88:A:VAL:HG12	1:93:A:ALA:HB2	13	1.28
(1,1335)	1:88:A:VAL:HG12	1:93:A:ALA:HB3	13	1.28
(1,1335)	1:88:A:VAL:HG13	1:93:A:ALA:HB1	13	1.28
(1,1335)	1:88:A:VAL:HG13	1:93:A:ALA:HB2	13	1.28
(1,1335)	1:88:A:VAL:HG13	1:93:A:ALA:HB3	13	1.28
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	5	1.28
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	5	1.28
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	5	1.28
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD2	18	1.28
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD3	18	1.28
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	1	1.28
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	6	1.27
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	6	1.27
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	6	1.27
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	6	1.27
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	6	1.27
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	6	1.27
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	6	1.27
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	6	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	6	1.27
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	10	1.27
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	10	1.27
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	10	1.27
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	18	1.27
(1,2937)	1:16:A:VAL:HG11	1:107:A:LEU:H	6	1.27
(1,2937)	1:16:A:VAL:HG12	1:107:A:LEU:H	6	1.27
(1,2937)	1:16:A:VAL:HG13	1:107:A:LEU:H	6	1.27
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	7	1.27
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	8	1.27
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	11	1.27
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	13	1.27
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	15	1.27
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	14	1.27
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	10	1.27
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	10	1.27
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	2	1.27
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	2	1.27
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	2	1.27
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD2	7	1.27
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD3	7	1.27
(1,193)	1:16:A:VAL:HG11	1:17:A:GLU:HA	6	1.27
(1,193)	1:16:A:VAL:HG12	1:17:A:GLU:HA	6	1.27
(1,193)	1:16:A:VAL:HG13	1:17:A:GLU:HA	6	1.27
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	14	1.26
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	19	1.26
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	11	1.26
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	16	1.26
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	1	1.26
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	12	1.26
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	18	1.26
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	4	1.26
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	3	1.26
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	3	1.26
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	3	1.26
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	11	1.26
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	11	1.26
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	7	1.26
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	7	1.26
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	7	1.26
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	14	1.26
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	17	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	8	1.25
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	8	1.25
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	8	1.25
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	8	1.25
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	8	1.25
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	8	1.25
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	8	1.25
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	8	1.25
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	8	1.25
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	15	1.25
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	15	1.25
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	15	1.25
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	8	1.25
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	3	1.25
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	8	1.25
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	11	1.25
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	3	1.25
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	14	1.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	11	1.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	11	1.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	11	1.25
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	2	1.25
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	2	1.25
(1,193)	1:16:A:VAL:HG11	1:17:A:GLU:HA	17	1.25
(1,193)	1:16:A:VAL:HG12	1:17:A:GLU:HA	17	1.25
(1,193)	1:16:A:VAL:HG13	1:17:A:GLU:HA	17	1.25
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	16	1.24
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	17	1.24
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	10	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	4	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	4	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	4	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	7	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	7	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	7	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	9	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	9	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	9	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	13	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	13	1.24
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	13	1.24
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	3	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	3	1.24
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	3	1.24
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD2	9	1.24
(1,877)	1:95:A:LYS:HB3	1:96:A:ARG:HD3	9	1.24
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	14	1.24
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	15	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	14	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	14	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	14	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	18	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	18	1.23
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	18	1.23
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	19	1.23
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	19	1.23
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	19	1.23
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	8	1.23
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	8	1.23
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	8	1.23
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	15	1.23
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	10	1.22
(1,1633)	1:14:A:GLN:H	1:111:A:ARG:HD3	18	1.22
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	6	1.22
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	6	1.22
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	6	1.22
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	5	1.22
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	5	1.22
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	4	1.21
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG11	7	1.21
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG12	7	1.21
(1,3045)	1:32:A:SER:HB3	1:57:A:VAL:HG13	7	1.21
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	16	1.21
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	2	1.21
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	10	1.21
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	10	1.21
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	17	1.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	9	1.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	9	1.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	9	1.21
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	6	1.21
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	4	1.2
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	3	1.2
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	15	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	11	1.2
(1,658)	1:61:A:SER:HA	1:62:A:GLU:HB2	11	1.2
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	6	1.19
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	6	1.19
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	14	1.19
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	1	1.18
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	1	1.18
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	1	1.18
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	1	1.18
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	1	1.18
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	1	1.18
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	1	1.18
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	1	1.18
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	1	1.18
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	13	1.18
(1,3066)	1:52:A:ASP:HB3	1:54:A:GLY:HA3	11	1.18
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	4	1.18
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	4	1.18
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	4	1.18
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	8	1.18
(1,1890)	1:31:A:PHE:H	1:32:A:SER:HA	18	1.18
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG21	6	1.18
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG22	6	1.18
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG23	6	1.18
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	3	1.18
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	1	1.18
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	1	1.18
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	1	1.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	11	1.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	11	1.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	11	1.18
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	8	1.18
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	13	1.17
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	7	1.17
(1,1860)	1:27:A:LEU:H	1:28:A:ILE:HA	13	1.17
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	19	1.17
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	20	1.17
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	7	1.17
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	7	1.17
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	7	1.17
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	16	1.16
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	16	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	16	1.16
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	16	1.16
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	16	1.16
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	16	1.16
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	16	1.16
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	16	1.16
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	16	1.16
(1,2212)	1:60:A:VAL:HG11	1:63:A:GLY:H	7	1.16
(1,2212)	1:60:A:VAL:HG12	1:63:A:GLY:H	7	1.16
(1,2212)	1:60:A:VAL:HG13	1:63:A:GLY:H	7	1.16
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	16	1.16
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	2	1.16
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	10	1.16
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	18	1.16
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	16	1.15
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	10	1.15
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	8	1.15
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	8	1.15
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	8	1.15
(1,1327)	1:88:A:VAL:HG11	1:93:A:ALA:HA	13	1.15
(1,1327)	1:88:A:VAL:HG12	1:93:A:ALA:HA	13	1.15
(1,1327)	1:88:A:VAL:HG13	1:93:A:ALA:HA	13	1.15
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	20	1.15
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	20	1.14
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	17	1.14
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	18	1.14
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	4	1.14
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	13	1.14
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	13	1.14
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	13	1.14
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	19	1.14
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	19	1.14
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	19	1.14
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	16	1.14
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	8	1.14
(1,235)	1:21:A:LEU:HA	1:22:A:ARG:HB3	12	1.14
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	13	1.14
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	10	1.13
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	19	1.13
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	6	1.13
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	10	1.13
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	10	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	10	1.13
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	9	1.13
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	5	1.13
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	15	1.13
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	18	1.12
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	18	1.12
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	18	1.12
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	18	1.12
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	18	1.12
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	18	1.12
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	18	1.12
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	18	1.12
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	18	1.12
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	12	1.12
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	12	1.12
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	12	1.12
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	9	1.12
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	6	1.12
(1,2487)	1:88:A:VAL:HG11	1:92:A:GLN:H	13	1.12
(1,2487)	1:88:A:VAL:HG12	1:92:A:GLN:H	13	1.12
(1,2487)	1:88:A:VAL:HG13	1:92:A:GLN:H	13	1.12
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	2	1.12
(1,1758)	1:15:A:ARG:H	1:16:A:VAL:HA	17	1.12
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	13	1.12
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	12	1.12
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	14	1.12
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	11	1.12
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	13	1.11
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	11	1.11
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	13	1.11
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	3	1.11
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	4	1.11
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	20	1.11
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	5	1.11
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	13	1.1
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB1	17	1.1
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB2	17	1.1
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB3	17	1.1
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB1	17	1.1
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB2	17	1.1
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB3	17	1.1
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB1	17	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB2	17	1.1
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB3	17	1.1
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	16	1.1
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	16	1.1
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	19	1.1
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	11	1.09
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	11	1.09
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	11	1.09
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	5	1.09
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	13	1.09
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	4	1.09
(1,2244)	1:60:A:VAL:HG11	1:67:A:GLU:H	12	1.09
(1,2244)	1:60:A:VAL:HG12	1:67:A:GLU:H	12	1.09
(1,2244)	1:60:A:VAL:HG13	1:67:A:GLU:H	12	1.09
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	14	1.09
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	5	1.09
(1,1633)	1:14:A:GLN:H	1:111:A:ARG:HD3	4	1.09
(1,1620)	1:113:A:SER:HA	1:115:A:GLN:HB2	10	1.09
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	17	1.09
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	17	1.09
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	17	1.09
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	2	1.08
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	1	1.08
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	4	1.08
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	7	1.08
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	18	1.08
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	18	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	6	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	6	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	6	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	20	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	20	1.08
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	20	1.08
(1,944)	1:102:A:GLU:HA	1:103:A:GLU:HG2	1	1.08
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	6	1.08
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	6	1.08
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	7	1.07
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	7	1.07
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	7	1.07
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	7	1.07
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	7	1.07
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	7	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	7	1.07
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	7	1.07
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	7	1.07
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	8	1.07
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	8	1.07
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	8	1.07
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	17	1.07
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	7	1.07
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	15	1.07
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	18	1.07
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	14	1.07
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	14	1.07
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	14	1.07
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	14	1.07
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	1	1.07
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	7	1.07
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	2	1.06
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	2	1.06
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	2	1.06
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	11	1.06
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	18	1.06
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	2	1.06
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	8	1.06
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	8	1.06
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	8	1.06
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	8	1.06
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	19	1.06
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	10	1.06
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	10	1.06
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	10	1.06
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	20	1.06
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	2	1.05
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	16	1.05
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	3	1.05
(1,2285)	1:67:A:GLU:HG2	1:70:A:GLY:H	7	1.05
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	16	1.05
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB2	14	1.05
(1,1462)	1:41:A:PRO:HB3	1:42:A:SER:HB3	14	1.05
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	8	1.05
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	8	1.05
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	8	1.05
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	9	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	4	1.04
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	8	1.04
(1,1725)	1:79:A:GLN:HG3	1:80:A:VAL:H	13	1.04
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	2	1.04
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	19	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	4	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	4	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	4	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	11	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	11	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	11	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	16	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	16	1.04
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	16	1.04
(1,1245)	1:88:A:VAL:HG11	1:92:A:GLN:HB2	13	1.04
(1,1245)	1:88:A:VAL:HG12	1:92:A:GLN:HB2	13	1.04
(1,1245)	1:88:A:VAL:HG13	1:92:A:GLN:HB2	13	1.04
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	3	1.04
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	12	1.04
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	12	1.04
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	12	1.04
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	19	1.03
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	19	1.03
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	19	1.03
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	11	1.03
(1,1648)	1:109:A:VAL:HG11	1:110:A:THR:HB	14	1.03
(1,1648)	1:109:A:VAL:HG12	1:110:A:THR:HB	14	1.03
(1,1648)	1:109:A:VAL:HG13	1:110:A:THR:HB	14	1.03
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	7	1.03
(1,3066)	1:52:A:ASP:HB3	1:54:A:GLY:HA3	18	1.02
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	9	1.02
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	9	1.02
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	9	1.02
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	18	1.02
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	6	1.01
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	10	1.01
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	19	1.01
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	3	1.01
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	13	1.01
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	13	1.01
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	13	1.01
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	13	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	15	1.01
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	15	1.01
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	15	1.01
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	6	1.01
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	9	1.0
(1,2508)	1:88:A:VAL:HG11	1:93:A:ALA:H	13	1.0
(1,2508)	1:88:A:VAL:HG12	1:93:A:ALA:H	13	1.0
(1,2508)	1:88:A:VAL:HG13	1:93:A:ALA:H	13	1.0
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG21	17	1.0
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG22	17	1.0
(1,1684)	1:15:A:ARG:H	1:16:A:VAL:HG23	17	1.0
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	1	1.0
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	1	1.0
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	1	1.0
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	5	1.0
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	4	1.0
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	15	0.99
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	3	0.99
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	3	0.99
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	3	0.99
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	3	0.99
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	18	0.99
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	18	0.99
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	18	0.99
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	16	0.99
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	10	0.99
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	12	0.99
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	3	0.98
(1,1636)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	15	0.98
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	7	0.98
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	7	0.98
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	7	0.98
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	8	0.98
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	9	0.98
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	12	0.98
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	13	0.98
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	16	0.98
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	18	0.98
(2,53)	1:32:A:SER:H	1:58:A:THR:O	5	0.97
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	17	0.97
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	13	0.97
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	14	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	14	0.97
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	14	0.97
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG21	12	0.97
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG22	12	0.97
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG23	12	0.97
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	3	0.97
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	10	0.97
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	14	0.97
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	1	0.97
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	5	0.97
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	11	0.97
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	15	0.97
(2,59)	1:32:A:SER:N	1:58:A:THR:O	19	0.96
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	12	0.96
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	20	0.96
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	1	0.96
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	3	0.96
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	3	0.96
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	3	0.96
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	10	0.96
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	11	0.96
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	3	0.96
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	16	0.96
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	16	0.95
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	16	0.95
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	16	0.95
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	14	0.95
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	15	0.95
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	15	0.95
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	15	0.95
(1,2244)	1:60:A:VAL:HG11	1:67:A:GLU:H	7	0.95
(1,2244)	1:60:A:VAL:HG12	1:67:A:GLU:H	7	0.95
(1,2244)	1:60:A:VAL:HG13	1:67:A:GLU:H	7	0.95
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	17	0.95
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	17	0.95
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	17	0.95
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	5	0.95
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	5	0.95
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	5	0.95
(1,1040)	1:61:A:SER:HB2	1:62:A:GLU:HB2	7	0.95
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	19	0.95
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	10	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	1	0.94
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	8	0.94
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	13	0.94
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	6	0.94
(1,1647)	1:104:A:VAL:HB	1:106:A:ARG:HD3	5	0.94
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	8	0.94
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	8	0.94
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	8	0.94
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	19	0.94
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	19	0.94
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	19	0.94
(1,509)	1:49:A:ASP:HB2	1:50:A:LYS:HA	2	0.94
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	2	0.94
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	9	0.94
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	17	0.94
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	12	0.94
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	15	0.93
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	2	0.93
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	10	0.93
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	10	0.93
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	10	0.93
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	10	0.93
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	14	0.93
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	20	0.93
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	18	0.93
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	8	0.92
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	9	0.92
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	16	0.92
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	19	0.92
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	19	0.92
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	19	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	2	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	2	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	2	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	12	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	12	0.92
(1,1336)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	12	0.92
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	3	0.92
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	20	0.91
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	15	0.91
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	2	0.91
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	1	0.9
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	1	0.9
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	7	0.9
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	20	0.9
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	9	0.9
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	8	0.9
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	5	0.89
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	13	0.89
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	15	0.89
(2,53)	1:32:A:SER:H	1:58:A:THR:O	10	0.88
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	14	0.88
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	14	0.88
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	14	0.88
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	14	0.88
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	14	0.88
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	14	0.88
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	14	0.88
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	14	0.88
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	14	0.88
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	9	0.88
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	9	0.88
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	9	0.88
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	17	0.88
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	6	0.88
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	14	0.88
(1,222)	1:18:A:ILE:HA	1:19:A:HIS:HB3	6	0.88
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	14	0.87
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD11	16	0.87
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD12	16	0.87
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD13	16	0.87
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG21	7	0.87
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG22	7	0.87
(1,2181)	1:59:A:ARG:H	1:60:A:VAL:HG23	7	0.87
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	17	0.87
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	3	0.86
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	7	0.86
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	20	0.86
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	11	0.86
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	19	0.86
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	6	0.86
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	15	0.86
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	15	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	15	0.86
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	14	0.86
(1,683)	1:62:A:GLU:HB3	1:63:A:GLY:HA3	11	0.86
(2,53)	1:32:A:SER:H	1:58:A:THR:O	11	0.85
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	16	0.85
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	14	0.85
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	20	0.85
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	20	0.85
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	20	0.85
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	4	0.85
(1,2775)	1:14:A:GLN:H	1:109:A:VAL:HG11	14	0.85
(1,2775)	1:14:A:GLN:H	1:109:A:VAL:HG12	14	0.85
(1,2775)	1:14:A:GLN:H	1:109:A:VAL:HG13	14	0.85
(1,1962)	1:38:A:ASP:H	1:39:A:GLN:HG3	15	0.85
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	11	0.85
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	1	0.85
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	1	0.85
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	1	0.85
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	1	0.85
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	1	0.85
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	1	0.85
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	3	0.84
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	6	0.84
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	6	0.84
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	6	0.84
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	6	0.84
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	15	0.84
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD11	3	0.84
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD12	3	0.84
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD13	3	0.84
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	1	0.84
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	8	0.83
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	14	0.83
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	16	0.83
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	10	0.83
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	11	0.83
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	20	0.83
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	7	0.83
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	7	0.83
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	7	0.83
(2,53)	1:32:A:SER:H	1:58:A:THR:O	12	0.82
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	19	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	2	0.82
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	3	0.82
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	14	0.82
(1,2897)	1:79:A:GLN:HG3	1:82:A:GLY:H	13	0.82
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	7	0.82
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	6	0.82
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	6	0.82
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	6	0.82
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	5	0.81
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	10	0.81
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	10	0.81
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	8	0.81
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	11	0.81
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	2	0.8
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	4	0.8
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	18	0.8
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	4	0.8
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	15	0.8
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	15	0.8
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	15	0.8
(1,1303)	1:88:A:VAL:HG11	1:92:A:GLN:HA	13	0.8
(1,1303)	1:88:A:VAL:HG12	1:92:A:GLN:HA	13	0.8
(1,1303)	1:88:A:VAL:HG13	1:92:A:GLN:HA	13	0.8
(1,683)	1:62:A:GLU:HB3	1:63:A:GLY:HA3	16	0.8
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	6	0.79
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	16	0.79
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	10	0.79
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	20	0.79
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	20	0.79
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	20	0.79
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	13	0.79
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	19	0.79
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	19	0.79
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	20	0.79
(2,53)	1:32:A:SER:H	1:58:A:THR:O	16	0.78
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	1	0.78
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	3	0.78
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	17	0.78
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	15	0.78
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	2	0.78
(1,142)	1:13:A:VAL:HG11	1:14:A:GLN:HA	5	0.78
(1,142)	1:13:A:VAL:HG12	1:14:A:GLN:HA	5	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:13:A:VAL:HG13	1:14:A:GLN:HA	5	0.78
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	5	0.77
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	2	0.77
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	18	0.77
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	18	0.77
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	18	0.77
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	12	0.77
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	12	0.77
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	12	0.77
(1,1485)	1:60:A:VAL:HG21	1:73:A:ILE:HA	12	0.77
(1,1485)	1:60:A:VAL:HG22	1:73:A:ILE:HA	12	0.77
(1,1485)	1:60:A:VAL:HG23	1:73:A:ILE:HA	12	0.77
(1,1240)	1:88:A:VAL:HG11	1:93:A:ALA:HA	13	0.77
(1,1240)	1:88:A:VAL:HG12	1:93:A:ALA:HA	13	0.77
(1,1240)	1:88:A:VAL:HG13	1:93:A:ALA:HA	13	0.77
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	14	0.77
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	19	0.76
(2,53)	1:32:A:SER:H	1:58:A:THR:O	20	0.76
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	13	0.76
(1,3041)	1:31:A:PHE:HB2	1:66:A:ALA:H	19	0.76
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	1	0.76
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	6	0.76
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	7	0.76
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	12	0.76
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	14	0.76
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	1	0.76
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	1	0.76
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	17	0.76
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	17	0.76
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	14	0.75
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	20	0.75
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	17	0.75
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	17	0.75
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	17	0.75
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	4	0.75
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	13	0.75
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	8	0.75
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	3	0.75
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	14	0.75
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	12	0.74
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	5	0.74
(1,2980)	1:14:A:GLN:HE22	1:109:A:VAL:H	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	12	0.74
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	14	0.74
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	9	0.74
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	9	0.74
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	9	0.74
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	11	0.74
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	11	0.74
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	11	0.74
(1,1485)	1:60:A:VAL:HG21	1:73:A:ILE:HA	7	0.74
(1,1485)	1:60:A:VAL:HG22	1:73:A:ILE:HA	7	0.74
(1,1485)	1:60:A:VAL:HG23	1:73:A:ILE:HA	7	0.74
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	18	0.74
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	6	0.73
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	14	0.73
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	7	0.73
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	7	0.73
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	7	0.73
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	14	0.73
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	15	0.73
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	18	0.73
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	17	0.73
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	4	0.73
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	4	0.73
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	4	0.73
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	9	0.73
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	9	0.73
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	9	0.73
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	1	0.73
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	9	0.73
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	10	0.73
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	13	0.72
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	14	0.72
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	19	0.72
(1,2958)	1:72:A:GLN:HE22	1:111:A:ARG:H	12	0.72
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	5	0.72
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB2	5	0.72
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB3	5	0.72
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	18	0.71
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	3	0.71
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	18	0.71
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	16	0.71
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	15	0.71
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	9	0.71
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	7	0.71
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	9	0.71
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	4	0.71
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	13	0.71
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	15	0.71
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	15	0.71
(2,53)	1:32:A:SER:H	1:58:A:THR:O	18	0.7
(1,3128)	1:85:A:MET:HE1	1:92:A:GLN:HE22	13	0.7
(1,3128)	1:85:A:MET:HE2	1:92:A:GLN:HE22	13	0.7
(1,3128)	1:85:A:MET:HE3	1:92:A:GLN:HE22	13	0.7
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	19	0.7
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	8	0.7
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD11	8	0.7
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD12	8	0.7
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD13	8	0.7
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	3	0.7
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	6	0.7
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	9	0.69
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	7	0.69
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	10	0.69
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	1	0.69
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	4	0.69
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	7	0.69
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	5	0.69
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	16	0.69
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	6	0.69
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	12	0.69
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	17	0.69
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	17	0.68
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	7	0.68
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	18	0.68
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	2	0.68
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	13	0.68
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	13	0.68
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	13	0.68
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	10	0.68
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	7	0.68
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	7	0.68
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	7	0.68
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	18	0.68
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	18	0.68
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	10	0.68
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	12	0.68
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	12	0.68
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	7	0.67
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	8	0.67
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	11	0.67
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	18	0.67
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	7	0.67
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	9	0.67
(1,2835)	1:60:A:VAL:HG11	1:71:A:LEU:H	7	0.67
(1,2835)	1:60:A:VAL:HG12	1:71:A:LEU:H	7	0.67
(1,2835)	1:60:A:VAL:HG13	1:71:A:LEU:H	7	0.67
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	16	0.67
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	16	0.67
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	16	0.67
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	10	0.67
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	2	0.67
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	5	0.67
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	5	0.67
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	5	0.67
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	12	0.67
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	12	0.67
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	12	0.67
(1,142)	1:13:A:VAL:HG11	1:14:A:GLN:HA	19	0.67
(1,142)	1:13:A:VAL:HG12	1:14:A:GLN:HA	19	0.67
(1,142)	1:13:A:VAL:HG13	1:14:A:GLN:HA	19	0.67
(1,68)	1:6:A:GLY:HA3	1:7:A:GLN:HG2	15	0.67
(1,68)	1:6:A:GLY:HA3	1:7:A:GLN:HG3	15	0.67
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	2	0.66
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	16	0.66
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	5	0.66
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	13	0.66
(1,2980)	1:14:A:GLN:HE22	1:109:A:VAL:H	12	0.66
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	5	0.66
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	5	0.66
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	5	0.66
(1,2779)	1:14:A:GLN:HE22	1:16:A:VAL:HG11	17	0.66
(1,2779)	1:14:A:GLN:HE22	1:16:A:VAL:HG12	17	0.66
(1,2779)	1:14:A:GLN:HE22	1:16:A:VAL:HG13	17	0.66
(1,2311)	1:72:A:GLN:H	1:72:A:GLN:HE22	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	10	0.66
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	10	0.66
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	10	0.66
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	14	0.66
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	14	0.66
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	14	0.66
(1,1436)	1:14:A:GLN:HE22	1:16:A:VAL:HG11	17	0.66
(1,1436)	1:14:A:GLN:HE22	1:16:A:VAL:HG12	17	0.66
(1,1436)	1:14:A:GLN:HE22	1:16:A:VAL:HG13	17	0.66
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	8	0.66
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	8	0.66
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	8	0.66
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	8	0.66
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	8	0.66
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	8	0.66
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	2	0.66
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	13	0.66
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	14	0.66
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	20	0.66
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	13	0.65
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	10	0.65
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	13	0.65
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	12	0.65
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	5	0.65
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	5	0.65
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	5	0.65
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	1	0.65
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	8	0.65
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	2	0.64
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	3	0.64
(2,53)	1:32:A:SER:H	1:58:A:THR:O	14	0.64
(1,3101)	1:91:A:ASP:HB3	1:95:A:LYS:HG2	15	0.64
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	14	0.64
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	17	0.64
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	15	0.64
(1,2466)	1:90:A:HIS:H	1:91:A:ASP:HB2	12	0.64
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	8	0.64
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	5	0.64
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	5	0.64
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	5	0.64
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	5	0.64
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	5	0.64
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	5	0.64
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	5	0.64
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	5	0.64
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	15	0.64
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	5	0.64
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	11	0.64
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	15	0.64
(1,3065)	1:52:A:ASP:HB3	1:54:A:GLY:H	11	0.63
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	13	0.63
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	9	0.63
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	9	0.63
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	9	0.63
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	13	0.63
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	13	0.63
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	13	0.63
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	16	0.63
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	16	0.63
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	16	0.63
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	19	0.63
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	19	0.63
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	19	0.63
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	19	0.63
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	19	0.63
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	19	0.63
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	19	0.63
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	19	0.63
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	19	0.63
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	18	0.63
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	18	0.63
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	3	0.63
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	10	0.63
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	17	0.62
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	6	0.62
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	10	0.62
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	16	0.62
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	16	0.62
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	20	0.62
(1,3014)	1:92:A:GLN:H	1:92:A:GLN:HE22	12	0.62
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	16	0.62
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	11	0.62
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	11	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	11	0.62
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	11	0.62
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	11	0.62
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	11	0.62
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	11	0.62
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	11	0.62
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	11	0.62
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	1	0.62
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	11	0.62
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	11	0.62
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	11	0.62
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	13	0.61
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	19	0.61
(1,2689)	1:111:A:ARG:HG3	1:113:A:SER:H	18	0.61
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	12	0.61
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	14	0.61
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	1	0.61
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	5	0.61
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	7	0.61
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	14	0.61
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	14	0.61
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	14	0.61
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	5	0.6
(1,2081)	1:48:A:GLU:H	1:52:A:ASP:HB2	18	0.6
(1,1988)	1:36:A:GLY:HA2	1:39:A:GLN:HE21	19	0.6
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	10	0.6
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	4	0.6
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	4	0.6
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	4	0.6
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	5	0.6
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	5	0.6
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	5	0.6
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	15	0.6
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	9	0.59
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	13	0.59
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	14	0.59
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	19	0.59
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	19	0.59
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	19	0.59
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	19	0.59
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	19	0.59
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:107:A:LEU:HG	1:109:A:VAL:HG21	14	0.59
(1,1003)	1:107:A:LEU:HG	1:109:A:VAL:HG22	14	0.59
(1,1003)	1:107:A:LEU:HG	1:109:A:VAL:HG23	14	0.59
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	6	0.59
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	8	0.59
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	7	0.59
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	12	0.58
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	1	0.58
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG11	10	0.58
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG12	10	0.58
(1,3048)	1:32:A:SER:H	1:57:A:VAL:HG13	10	0.58
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	1	0.58
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	10	0.58
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	11	0.58
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	17	0.58
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	11	0.58
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	3	0.58
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	3	0.58
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	3	0.58
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	19	0.58
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	5	0.58
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	20	0.58
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	20	0.58
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	20	0.58
(1,141)	1:13:A:VAL:HG11	1:14:A:GLN:H	11	0.58
(1,141)	1:13:A:VAL:HG12	1:14:A:GLN:H	11	0.58
(1,141)	1:13:A:VAL:HG13	1:14:A:GLN:H	11	0.58
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	16	0.57
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	13	0.57
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	20	0.57
(1,2697)	1:112:A:GLN:HG3	1:114:A:LEU:H	19	0.57
(1,2466)	1:90:A:HIS:H	1:91:A:ASP:HB2	17	0.57
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	1	0.57
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	1	0.57
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	1	0.57
(1,1241)	1:88:A:VAL:HG11	1:93:A:ALA:HB1	13	0.57
(1,1241)	1:88:A:VAL:HG11	1:93:A:ALA:HB2	13	0.57
(1,1241)	1:88:A:VAL:HG11	1:93:A:ALA:HB3	13	0.57
(1,1241)	1:88:A:VAL:HG12	1:93:A:ALA:HB1	13	0.57
(1,1241)	1:88:A:VAL:HG12	1:93:A:ALA:HB2	13	0.57
(1,1241)	1:88:A:VAL:HG12	1:93:A:ALA:HB3	13	0.57
(1,1241)	1:88:A:VAL:HG13	1:93:A:ALA:HB1	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:88:A:VAL:HG13	1:93:A:ALA:HB2	13	0.57
(1,1241)	1:88:A:VAL:HG13	1:93:A:ALA:HB3	13	0.57
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	20	0.57
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	3	0.57
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	20	0.57
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	7	0.57
(1,179)	1:15:A:ARG:HB3	1:16:A:VAL:HA	11	0.57
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	12	0.57
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	12	0.57
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	12	0.57
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	3	0.56
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	11	0.56
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	6	0.56
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	7	0.56
(1,2809)	1:23:A:GLN:HE22	1:28:A:ILE:HG21	10	0.56
(1,2809)	1:23:A:GLN:HE22	1:28:A:ILE:HG22	10	0.56
(1,2809)	1:23:A:GLN:HE22	1:28:A:ILE:HG23	10	0.56
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	2	0.56
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	13	0.56
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	14	0.56
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	20	0.56
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	7	0.56
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	7	0.56
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	8	0.56
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	8	0.56
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	8	0.56
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	4	0.56
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	9	0.56
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	4	0.56
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	16	0.56
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	16	0.56
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	16	0.56
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	8	0.56
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	8	0.56
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	8	0.56
(1,142)	1:13:A:VAL:HG11	1:14:A:GLN:HA	11	0.56
(1,142)	1:13:A:VAL:HG12	1:14:A:GLN:HA	11	0.56
(1,142)	1:13:A:VAL:HG13	1:14:A:GLN:HA	11	0.56
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB2	11	0.56
(1,2)	1:40:A:ASP:HB3	1:42:A:SER:HB3	11	0.56
(1,2986)	1:72:A:GLN:HE22	1:113:A:SER:H	12	0.55
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	7	0.55
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	1	0.55
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	8	0.55
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	19	0.55
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	19	0.55
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	19	0.55
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	19	0.55
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	19	0.55
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	19	0.55
(1,1008)	1:109:A:VAL:HG11	1:110:A:THR:HA	14	0.55
(1,1008)	1:109:A:VAL:HG12	1:110:A:THR:HA	14	0.55
(1,1008)	1:109:A:VAL:HG13	1:110:A:THR:HA	14	0.55
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	12	0.55
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	9	0.54
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	14	0.54
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	2	0.54
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	2	0.54
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	2	0.54
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	12	0.54
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	11	0.54
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	15	0.54
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	3	0.54
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	3	0.54
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	4	0.54
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	4	0.54
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	7	0.54
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	7	0.54
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	7	0.54
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	5	0.54
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	5	0.54
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	5	0.54
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	15	0.54
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	15	0.54
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	15	0.54
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	12	0.54
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	12	0.54
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	17	0.54
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	3	0.54
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	12	0.54
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	12	0.54
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	12	0.54
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	12	0.54
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	12	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	12	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	12	0.54
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	12	0.54
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	7	0.54
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	11	0.53
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	9	0.53
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	18	0.53
(1,2697)	1:112:A:GLN:HG3	1:114:A:LEU:H	15	0.53
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	3	0.53
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	10	0.53
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	18	0.53
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	18	0.53
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	1	0.53
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	1	0.53
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	1	0.53
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	11	0.53
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	11	0.53
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	11	0.53
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	15	0.53
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	19	0.53
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB1	7	0.53
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB2	7	0.53
(1,638)	1:60:A:VAL:HG11	1:66:A:ALA:HB3	7	0.53
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB1	7	0.53
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB2	7	0.53
(1,638)	1:60:A:VAL:HG12	1:66:A:ALA:HB3	7	0.53
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB1	7	0.53
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB2	7	0.53
(1,638)	1:60:A:VAL:HG13	1:66:A:ALA:HB3	7	0.53
(1,3112)	1:36:A:GLY:HA2	1:91:A:ASP:H	15	0.52
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	4	0.52
(1,2955)	1:13:A:VAL:HG21	1:111:A:ARG:H	5	0.52
(1,2955)	1:13:A:VAL:HG22	1:111:A:ARG:H	5	0.52
(1,2955)	1:13:A:VAL:HG23	1:111:A:ARG:H	5	0.52
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	7	0.52
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	7	0.52
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	7	0.52
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	7	0.52
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	15	0.52
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	15	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	15	0.52
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	5	0.52
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	3	0.52
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	3	0.52
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	3	0.52
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	18	0.52
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	18	0.52
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	18	0.52
(1,958)	1:103:A:GLU:HG3	1:104:A:VAL:HG11	17	0.52
(1,958)	1:103:A:GLU:HG3	1:104:A:VAL:HG12	17	0.52
(1,958)	1:103:A:GLU:HG3	1:104:A:VAL:HG13	17	0.52
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	16	0.52
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	20	0.52
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	20	0.52
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	20	0.52
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	16	0.51
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	10	0.51
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	2	0.51
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	2	0.51
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	2	0.51
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	2	0.51
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	2	0.51
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	2	0.51
(1,2717)	1:116:A:LYS:H	1:116:A:LYS:HB3	17	0.51
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	19	0.51
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	11	0.51
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	1	0.51
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	5	0.51
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	7	0.51
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	2	0.51
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	2	0.51
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	2	0.51
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	16	0.51
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	16	0.51
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	20	0.51
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	16	0.51
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	16	0.51
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	16	0.51
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	13	0.51
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	3	0.51
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	16	0.51
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	16	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	16	0.51
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	17	0.51
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	17	0.51
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	17	0.51
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	8	0.5
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	13	0.5
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	7	0.5
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	3	0.5
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	12	0.5
(1,2533)	1:91:A:ASP:HB3	1:95:A:LYS:H	12	0.5
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	11	0.5
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	20	0.5
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	20	0.5
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	20	0.5
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	1	0.5
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	8	0.5
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	18	0.5
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	18	0.5
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	18	0.5
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	12	0.5
(1,141)	1:13:A:VAL:HG11	1:14:A:GLN:H	19	0.5
(1,141)	1:13:A:VAL:HG12	1:14:A:GLN:H	19	0.5
(1,141)	1:13:A:VAL:HG13	1:14:A:GLN:H	19	0.5
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	2	0.49
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	12	0.49
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	3	0.49
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	7	0.49
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	11	0.49
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	20	0.49
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	1	0.49
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	1	0.49
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	1	0.49
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	15	0.49
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	15	0.49
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	15	0.49
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	5	0.49
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	7	0.49
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	15	0.49
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	15	0.49
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	15	0.49
(1,1437)	1:16:A:VAL:HG11	1:107:A:LEU:H	17	0.49
(1,1437)	1:16:A:VAL:HG12	1:107:A:LEU:H	17	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:16:A:VAL:HG13	1:107:A:LEU:H	17	0.49
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	8	0.49
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	8	0.49
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	8	0.49
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	3	0.49
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	3	0.49
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	3	0.49
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	3	0.49
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	3	0.49
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	3	0.49
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	11	0.49
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	11	0.49
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	20	0.49
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	20	0.49
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	20	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	8	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	8	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	8	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	11	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	11	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	11	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	17	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	17	0.49
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	17	0.49
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	18	0.49
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	18	0.49
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	18	0.49
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	11	0.49
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	17	0.49
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	13	0.48
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	20	0.48
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	10	0.48
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	13	0.48
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	13	0.48
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	13	0.48
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	19	0.48
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	12	0.48
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	6	0.48
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	14	0.48
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	14	0.48
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	14	0.48
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	16	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	16	0.48
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	16	0.48
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	16	0.48
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	16	0.48
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	16	0.48
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	6	0.48
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	6	0.48
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	20	0.48
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	20	0.48
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	20	0.48
(2,59)	1:32:A:SER:N	1:58:A:THR:O	5	0.47
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	15	0.47
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	12	0.47
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	13	0.47
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	13	0.47
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	13	0.47
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	13	0.47
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	13	0.47
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	13	0.47
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	13	0.47
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	13	0.47
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	13	0.47
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	2	0.47
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	20	0.47
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	8	0.47
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	15	0.47
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	7	0.47
(1,2912)	1:83:A:TRP:HE1	1:96:A:ARG:HB2	9	0.47
(1,2912)	1:83:A:TRP:HE1	1:96:A:ARG:HB2	18	0.47
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	6	0.47
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	6	0.47
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	6	0.47
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	17	0.47
(1,2572)	1:99:A:LYS:H	1:99:A:LYS:HG3	13	0.47
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	11	0.47
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	18	0.47
(1,1738)	1:13:A:VAL:HG11	1:14:A:GLN:H	11	0.47
(1,1738)	1:13:A:VAL:HG12	1:14:A:GLN:H	11	0.47
(1,1738)	1:13:A:VAL:HG13	1:14:A:GLN:H	11	0.47
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	12	0.47
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	12	0.47
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	9	0.47
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	9	0.47
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	18	0.47
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	5	0.47
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	16	0.47
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	11	0.47
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	11	0.47
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	11	0.47
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	4	0.46
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	5	0.46
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	11	0.46
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	8	0.46
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	3	0.46
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	3	0.46
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	16	0.46
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	2	0.46
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	2	0.46
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	2	0.46
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	17	0.46
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	17	0.46
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	17	0.46
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	16	0.46
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	16	0.46
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	16	0.46
(1,2533)	1:91:A:ASP:HB3	1:95:A:LYS:H	17	0.46
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	19	0.46
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	19	0.46
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	19	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	2	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	6	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	9	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	14	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	15	0.46
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	20	0.46
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	9	0.45
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	10	0.45
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	8	0.45
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	17	0.45
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	16	0.45
(1,3093)	1:24:A:GLY:HA2	1:25:A:GLU:HG3	13	0.45
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	4	0.45
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	5	0.45
(1,2903)	1:79:A:GLN:HB2	1:83:A:TRP:H	13	0.45
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	9	0.45
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	9	0.45
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	9	0.45
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	20	0.45
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	20	0.45
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	20	0.45
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	2	0.45
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	4	0.45
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	4	0.45
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	4	0.45
(1,1437)	1:16:A:VAL:HG11	1:107:A:LEU:H	6	0.45
(1,1437)	1:16:A:VAL:HG12	1:107:A:LEU:H	6	0.45
(1,1437)	1:16:A:VAL:HG13	1:107:A:LEU:H	6	0.45
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	10	0.45
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	10	0.45
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	10	0.45
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	10	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	10	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	10	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	10	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	13	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	13	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	13	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	15	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	15	0.45
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	15	0.45
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	16	0.45
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	11	0.45
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	20	0.45
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	12	0.45
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	19	0.45
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	2	0.45
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	2	0.45
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	2	0.45
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	3	0.45
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	3	0.45
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	3	0.45
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	3	0.45
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	3	0.45
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	19	0.44
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	19	0.44
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	19	0.44
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	19	0.44
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	19	0.44
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	19	0.44
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	19	0.44
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	19	0.44
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	19	0.44
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	15	0.44
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	1	0.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	2	0.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	2	0.44
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	2	0.44
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	15	0.44
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	10	0.44
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	10	0.44
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	10	0.44
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	10	0.44
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	7	0.44
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	7	0.44
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	7	0.44
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	10	0.44
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	10	0.44
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	10	0.44
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	3	0.44
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	3	0.44
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	3	0.44
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	10	0.44
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	2	0.44
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	2	0.44
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	2	0.44
(1,1535)	1:77:A:ILE:HA	1:109:A:VAL:HG21	14	0.44
(1,1535)	1:77:A:ILE:HA	1:109:A:VAL:HG22	14	0.44
(1,1535)	1:77:A:ILE:HA	1:109:A:VAL:HG23	14	0.44
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	4	0.44
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	4	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	2	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	2	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	2	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	5	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	5	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	14	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	14	0.44
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	14	0.44
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	9	0.44
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	1	0.44
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	7	0.44
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	15	0.43
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	5	0.43
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	1	0.43
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	7	0.43
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	5	0.43
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	13	0.43
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	17	0.43
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	4	0.43
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	4	0.43
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	4	0.43
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	4	0.43
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	4	0.43
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	4	0.43
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	14	0.43
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	14	0.43
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	14	0.43
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	18	0.43
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	18	0.43
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	18	0.43
(1,2311)	1:72:A:GLN:H	1:72:A:GLN:HE22	1	0.43
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	9	0.43
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	9	0.43
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	19	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	7	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	7	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	7	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	12	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	12	0.43
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	12	0.43
(1,659)	1:61:A:SER:HA	1:62:A:GLU:HG2	7	0.43
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	13	0.43
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	9	0.43
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	18	0.43
(1,55)	1:4:A:ILE:HB	1:5:A:PRO:HD3	12	0.43
(1,10)	1:39:A:GLN:HB2	1:40:A:ASP:HB3	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:39:A:GLN:HB3	1:40:A:ASP:HB3	14	0.43
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	1	0.42
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	5	0.42
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	5	0.42
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	5	0.42
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	5	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	3	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	3	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	3	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	3	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	3	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	3	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	3	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	3	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	3	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	10	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	10	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	10	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	10	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	10	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	10	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	10	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	10	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	10	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	17	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	17	0.42
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	17	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	17	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	17	0.42
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	17	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	17	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	17	0.42
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	17	0.42
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	1	0.42
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	18	0.42
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	18	0.42
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	18	0.42
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	19	0.42
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	20	0.42
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	11	0.42
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	4	0.42
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	16	0.42
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	15	0.42
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	15	0.42
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	15	0.42
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	13	0.42
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	8	0.42
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	6	0.42
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	14	0.42
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	7	0.42
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	10	0.42
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	10	0.42
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	10	0.42
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	13	0.42
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	13	0.42
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	13	0.42
(1,1176)	1:79:A:GLN:HG3	1:80:A:VAL:H	13	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	1	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	1	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	1	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	4	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	4	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	4	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	9	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	9	0.42
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	9	0.42
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	20	0.42
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	10	0.42
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	10	0.42
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	7	0.42
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	7	0.42
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	7	0.42
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	15	0.41
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	18	0.41
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	12	0.41
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	17	0.41
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	1	0.41
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	16	0.41
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	14	0.41
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	16	0.41
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	11	0.41
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	20	0.41
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	3	0.41
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG21	19	0.41
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG22	19	0.41
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG23	19	0.41
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	4	0.41
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	4	0.41
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	4	0.41
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	2	0.41
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	11	0.41
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	13	0.41
(1,1657)	1:64:A:GLY:HA2	1:65:A:PRO:HB3	19	0.41
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	4	0.41
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	4	0.41
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	4	0.41
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	4	0.41
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	4	0.41
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	4	0.41
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	17	0.41
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	17	0.41
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	17	0.41
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	10	0.41
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	14	0.41
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	16	0.41
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	3	0.41
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	3	0.41
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	3	0.41
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB1	6	0.41
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:65:A:PRO:HA	1:66:A:ALA:HB3	6	0.41
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	14	0.41
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	14	0.41
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	14	0.41
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	4	0.41
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	8	0.41
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	2	0.41
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	7	0.4
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	7	0.4
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	7	0.4
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	7	0.4
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	7	0.4
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	7	0.4
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	7	0.4
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	7	0.4
(1,3025)	1:32:A:SER:HB3	1:60:A:VAL:H	2	0.4
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	10	0.4
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	1	0.4
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	8	0.4
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	13	0.4
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	13	0.4
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	5	0.4
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	5	0.4
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	5	0.4
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	5	0.4
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	5	0.4
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	5	0.4
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	3	0.4
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	15	0.4
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	12	0.4
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	1	0.4
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	14	0.4
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	14	0.4
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	5	0.4
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	5	0.4
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	5	0.4
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	18	0.4
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	18	0.4
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	18	0.4
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	1	0.4
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	14	0.4
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	14	0.4
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	14	0.4
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	11	0.4
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	11	0.4
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	11	0.4
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	11	0.4
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	3	0.4
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	16	0.4
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	16	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	3	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	5	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	8	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	14	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	18	0.4
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	19	0.4
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	9	0.39
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	10	0.39
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	4	0.39
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	5	0.39
(1,3111)	1:78:A:MET:HA	1:108:A:LEU:H	6	0.39
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	13	0.39
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	8	0.39
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	8	0.39
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	8	0.39
(1,3047)	1:35:A:GLY:H	1:39:A:GLN:HG2	19	0.39
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	9	0.39
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	10	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	2	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	2	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	11	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	11	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	12	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	15	0.39
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	15	0.39
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	3	0.39
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	18	0.39
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	13	0.39
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	13	0.39
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	13	0.39
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	1	0.39
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	4	0.39
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	3	0.39
(1,1738)	1:13:A:VAL:HG11	1:14:A:GLN:H	19	0.39
(1,1738)	1:13:A:VAL:HG12	1:14:A:GLN:H	19	0.39
(1,1738)	1:13:A:VAL:HG13	1:14:A:GLN:H	19	0.39
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	16	0.39
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	16	0.39
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	20	0.39
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	1	0.39
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	1	0.39
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	10	0.39
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	10	0.39
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	14	0.39
(1,264)	1:24:A:GLY:HA3	1:25:A:GLU:HB3	10	0.39
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	1	0.39
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	1	0.39
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	1	0.39
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	4	0.39
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	5	0.39
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	5	0.39
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	5	0.39
(2,59)	1:32:A:SER:N	1:58:A:THR:O	10	0.38
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	5	0.38
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	15	0.38
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	20	0.38
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	4	0.38
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	6	0.38
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	8	0.38
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	8	0.38
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	8	0.38
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	19	0.38
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	8	0.38
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	16	0.38
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	16	0.38
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD11	15	0.38
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD12	15	0.38
(1,2843)	1:72:A:GLN:HE21	1:114:A:LEU:HD13	15	0.38
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	5	0.38
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	5	0.38
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	5	0.38
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	5	0.38
(1,2572)	1:99:A:LYS:H	1:99:A:LYS:HG3	7	0.38
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	18	0.38
(1,2129)	1:53:A:LYS:H	1:54:A:GLY:HA3	9	0.38
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	4	0.38
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	10	0.38
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	6	0.38
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	6	0.38
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	6	0.38
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	18	0.38
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	18	0.38
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	18	0.38
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	6	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	6	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	6	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	6	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	17	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	17	0.38
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	17	0.38
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	3	0.38
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	3	0.38
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	3	0.38
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	12	0.38
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	12	0.38
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	12	0.38
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	19	0.38
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	19	0.38
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	19	0.38
(1,141)	1:13:A:VAL:HG11	1:14:A:GLN:H	5	0.38
(1,141)	1:13:A:VAL:HG12	1:14:A:GLN:H	5	0.38
(1,141)	1:13:A:VAL:HG13	1:14:A:GLN:H	5	0.38
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	9	0.38
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	11	0.37
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	12	0.37
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	12	0.37
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	12	0.37
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	17	0.37
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	18	0.37
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	18	0.37
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	18	0.37
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	18	0.37
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	6	0.37
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	16	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	1	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	1	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	7	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	7	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	9	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	9	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	19	0.37
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	19	0.37
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	16	0.37
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	16	0.37
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	16	0.37
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	14	0.37
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	14	0.37
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	14	0.37
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	2	0.37
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	2	0.37
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	2	0.37
(1,2594)	1:99:A:LYS:HG3	1:102:A:GLU:H	16	0.37
(1,2572)	1:99:A:LYS:H	1:99:A:LYS:HG3	4	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	3	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	3	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	3	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	9	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	9	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	9	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	18	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	18	0.37
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	18	0.37
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	4	0.37
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	13	0.37
(1,511)	1:47:A:SER:HB2	1:52:A:ASP:HB2	1	0.37
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	6	0.37
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	6	0.37
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	6	0.37
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	20	0.37
(2,59)	1:32:A:SER:N	1:58:A:THR:O	11	0.36
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	3	0.36
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	10	0.36
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	10	0.36
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	13	0.36
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	13	0.36
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	11	0.36
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	11	0.36
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	11	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	1	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	1	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	1	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	4	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	4	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	4	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	6	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	6	0.36
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	6	0.36
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	1	0.36
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	10	0.36
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	11	0.36
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	14	0.36
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	5	0.36
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	5	0.36
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	4	0.36
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	4	0.36
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	5	0.36
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	5	0.36
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	19	0.36
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	4	0.36
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	4	0.36
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	4	0.36
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	17	0.36
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	17	0.36
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	17	0.36
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	10	0.36
(1,2721)	1:116:A:LYS:HA	1:117:A:ALA:H	6	0.36
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	7	0.36
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	7	0.36
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	7	0.36
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	15	0.36
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	15	0.36
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	15	0.36
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	20	0.36
(1,1992)	1:39:A:GLN:HA	1:39:A:GLN:HE22	19	0.36
(1,1591)	1:85:A:MET:HE1	1:92:A:GLN:HE22	15	0.36
(1,1591)	1:85:A:MET:HE2	1:92:A:GLN:HE22	15	0.36
(1,1591)	1:85:A:MET:HE3	1:92:A:GLN:HE22	15	0.36
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	1	0.36
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	7	0.36
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	13	0.36
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	16	0.36
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	13	0.36
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	13	0.36
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	13	0.36
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	13	0.36
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	13	0.36
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	13	0.36
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	4	0.36
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	4	0.36
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	4	0.36
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	7	0.36
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	5	0.36
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	2	0.36
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	4	0.36
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	4	0.36
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	4	0.36
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	11	0.36
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	2	0.35
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	9	0.35
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	18	0.35
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	16	0.35
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	16	0.35
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	16	0.35
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	18	0.35
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	11	0.35
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	11	0.35
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	2	0.35
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	17	0.35
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	20	0.35
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	3	0.35
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	3	0.35
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	13	0.35
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	1	0.35
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	1	0.35
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	1	0.35
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	16	0.35
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	8	0.35
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	9	0.35
(1,2012)	1:40:A:ASP:H	1:41:A:PRO:HD2	1	0.35
(1,1650)	1:112:A:GLN:HG3	1:113:A:SER:HA	12	0.35
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD11	9	0.35
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD12	9	0.35
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD13	9	0.35
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	15	0.35
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	17	0.35
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	17	0.35
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	11	0.35
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	2	0.35
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	2	0.35
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	2	0.35
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	2	0.35
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	19	0.35
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	19	0.35
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	7	0.34
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	13	0.34
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	16	0.34
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	2	0.34
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	2	0.34
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	2	0.34
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	6	0.34
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	13	0.34
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	12	0.34
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	2	0.34
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	5	0.34
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	20	0.34
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	20	0.34
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	20	0.34
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	4	0.34
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	6	0.34
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	6	0.34
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	17	0.34
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	17	0.34
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	18	0.34
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	18	0.34
(1,2909)	1:81:A:ASN:HB3	1:83:A:TRP:HE1	5	0.34
(1,2909)	1:81:A:ASN:HB3	1:83:A:TRP:HE1	6	0.34
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	11	0.34
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	11	0.34
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	11	0.34
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	11	0.34
(1,2845)	1:60:A:VAL:HG21	1:73:A:ILE:H	12	0.34
(1,2845)	1:60:A:VAL:HG22	1:73:A:ILE:H	12	0.34
(1,2845)	1:60:A:VAL:HG23	1:73:A:ILE:H	12	0.34
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	9	0.34
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	16	0.34
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	3	0.34
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	3	0.34
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	3	0.34
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	17	0.34
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	17	0.34
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	17	0.34
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	9	0.34
(1,2005)	1:39:A:GLN:HE21	1:40:A:ASP:H	19	0.34
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	13	0.34
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	13	0.34
(1,1628)	1:16:A:VAL:HG11	1:70:A:GLY:HA2	11	0.34
(1,1628)	1:16:A:VAL:HG12	1:70:A:GLY:HA2	11	0.34
(1,1628)	1:16:A:VAL:HG13	1:70:A:GLY:HA2	11	0.34
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	17	0.34
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD11	18	0.34
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD12	18	0.34
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD13	18	0.34
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	7	0.34
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	7	0.34
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	7	0.34
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	19	0.34
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	17	0.34
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	17	0.34
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	1	0.34
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	12	0.34
(2,59)	1:32:A:SER:N	1:58:A:THR:O	12	0.33
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	14	0.33
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	17	0.33
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	5	0.33
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	6	0.33
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	1	0.33
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	2	0.33
(1,3093)	1:24:A:GLY:HA2	1:25:A:GLU:HG3	4	0.33
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	14	0.33
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	14	0.33
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	14	0.33
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	14	0.33
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	12	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	14	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	14	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	14	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	15	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	15	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	15	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	16	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	16	0.33
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	16	0.33
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	19	0.33
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	7	0.33
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	13	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	10	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	10	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	14	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	14	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG2	20	0.33
(1,2971)	1:92:A:GLN:H	1:92:A:GLN:HG3	20	0.33
(1,2852)	1:56:A:TYR:HD1	1:75:A:ASP:H	20	0.33
(1,2852)	1:56:A:TYR:HD2	1:75:A:ASP:H	20	0.33
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	20	0.33
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	8	0.33
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	19	0.33
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	19	0.33
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	19	0.33
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	9	0.33
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	9	0.33
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	8	0.33
(1,2220)	1:62:A:GLU:HB3	1:63:A:GLY:H	16	0.33
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	17	0.33
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	9	0.33
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	8	0.33
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	12	0.33
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	20	0.33
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	20	0.33
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	16	0.33
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	6	0.33
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	7	0.33
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	7	0.32
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	7	0.32
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	7	0.32
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	8	0.32
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	8	0.32
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	8	0.32
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	20	0.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE1	5	0.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE2	5	0.32
(1,3130)	1:77:A:ILE:HG21	1:85:A:MET:HE3	5	0.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE1	5	0.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE2	5	0.32
(1,3130)	1:77:A:ILE:HG22	1:85:A:MET:HE3	5	0.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE1	5	0.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE2	5	0.32
(1,3130)	1:77:A:ILE:HG23	1:85:A:MET:HE3	5	0.32
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	3	0.32
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	3	0.32
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	3	0.32
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	18	0.32
(1,3095)	1:41:A:PRO:HB3	1:42:A:SER:HA	7	0.32
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	10	0.32
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	10	0.32
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	10	0.32
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	18	0.32
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	19	0.32
(1,2962)	1:36:A:GLY:HA2	1:91:A:ASP:H	8	0.32
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	2	0.32
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	14	0.32
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	18	0.32
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	18	0.32
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	7	0.32
(1,2012)	1:40:A:ASP:H	1:41:A:PRO:HD2	13	0.32
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	12	0.32
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	12	0.32
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	12	0.32
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	8	0.32
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	8	0.32
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	20	0.32
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	20	0.32
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	4	0.32
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	16	0.32
(1,670)	1:60:A:VAL:HG11	1:62:A:GLU:HA	12	0.32
(1,670)	1:60:A:VAL:HG12	1:62:A:GLU:HA	12	0.32
(1,670)	1:60:A:VAL:HG13	1:62:A:GLU:HA	12	0.32
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	8	0.32
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	8	0.32
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	18	0.32
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	12	0.31
(2,59)	1:32:A:SER:N	1:58:A:THR:O	16	0.31
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	4	0.31
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	6	0.31
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	13	0.31
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	13	0.31
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	13	0.31
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	9	0.31
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	9	0.31
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	9	0.31
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	7	0.31
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	7	0.31
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	7	0.31
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	5	0.31
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	9	0.31
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	9	0.31
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	9	0.31
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	14	0.31
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	14	0.31
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	14	0.31
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	17	0.31
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	17	0.31
(1,3074)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	17	0.31
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	6	0.31
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	2	0.31
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	2	0.31
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	2	0.31
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	9	0.31
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	14	0.31
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	14	0.31
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	14	0.31
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	18	0.31
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	18	0.31
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	18	0.31
(1,2852)	1:56:A:TYR:HD1	1:75:A:ASP:H	11	0.31
(1,2852)	1:56:A:TYR:HD2	1:75:A:ASP:H	11	0.31
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	10	0.31
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	10	0.31
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	10	0.31
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	10	0.31
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	18	0.31
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	18	0.31
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	18	0.31
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	15	0.31
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	2	0.31
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	3	0.31
(1,2220)	1:62:A:GLU:HB3	1:63:A:GLY:H	11	0.31
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	15	0.31
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	15	0.31
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	15	0.31
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	7	0.31
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	7	0.31
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	8	0.31
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	17	0.31
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	11	0.31
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	20	0.31
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	18	0.31
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	3	0.31
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	3	0.31
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	3	0.31
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	19	0.31
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	19	0.31
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	4	0.31
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	17	0.31
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	8	0.3
(2,59)	1:32:A:SER:N	1:58:A:THR:O	20	0.3
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	16	0.3
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	3	0.3
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	3	0.3
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	3	0.3
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	19	0.3
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	6	0.3
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	6	0.3
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	6	0.3
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	16	0.3
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	16	0.3
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	16	0.3
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	4	0.3
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	15	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	1	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	1	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	1	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	6	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	6	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	6	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	10	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	10	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	10	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	13	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	13	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	13	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	15	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	15	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	15	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	16	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	16	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	16	0.3
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	19	0.3
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	19	0.3
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	19	0.3
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	16	0.3
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	20	0.3
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	11	0.3
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	11	0.3
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	11	0.3
(1,3021)	1:115:A:GLN:HG2	1:117:A:ALA:H	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3021)	1:115:A:GLN:HG3	1:117:A:ALA:H	12	0.3
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	2	0.3
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	7	0.3
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	4	0.3
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	4	0.3
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	10	0.3
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	11	0.3
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	11	0.3
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	11	0.3
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	5	0.3
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	15	0.3
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	8	0.3
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	8	0.3
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	8	0.3
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	3	0.3
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	14	0.3
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	14	0.3
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	14	0.3
(1,2572)	1:99:A:LYS:H	1:99:A:LYS:HG3	10	0.3
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	4	0.3
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	4	0.3
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	4	0.3
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	20	0.3
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	16	0.3
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	16	0.3
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	19	0.3
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	20	0.3
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	3	0.3
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	3	0.3
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	3	0.3
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	3	0.3
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	3	0.3
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	3	0.3
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	3	0.3
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	3	0.3
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	3	0.3
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	10	0.3
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	10	0.3
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	10	0.3
(1,1486)	1:64:A:GLY:HA3	1:65:A:PRO:HB3	18	0.3
(1,1476)	1:58:A:THR:HG21	1:59:A:ARG:HG2	14	0.3
(1,1476)	1:58:A:THR:HG22	1:59:A:ARG:HG2	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:58:A:THR:HG23	1:59:A:ARG:HG2	14	0.3
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	14	0.3
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	14	0.3
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	14	0.3
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	11	0.3
(1,1375)	1:3:A:TYR:HE1	1:5:A:PRO:HD2	20	0.3
(1,1375)	1:3:A:TYR:HE2	1:5:A:PRO:HD2	20	0.3
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	12	0.3
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG2	7	0.3
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG3	7	0.3
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	9	0.3
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	9	0.3
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	9	0.3
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	19	0.3
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	10	0.3
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	14	0.3
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	8	0.3
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	12	0.3
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	16	0.3
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	2	0.29
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	2	0.29
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	2	0.29
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	15	0.29
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	15	0.29
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	15	0.29
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	5	0.29
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	5	0.29
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	5	0.29
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	10	0.29
(1,3156)	1:36:A:GLY:H	1:55:A:ILE:H	12	0.29
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	12	0.29
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	16	0.29
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	17	0.29
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	17	0.29
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	17	0.29
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	4	0.29
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	9	0.29
(1,3066)	1:52:A:ASP:HB3	1:54:A:GLY:HA3	2	0.29
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	2	0.29
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	18	0.29
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	9	0.29
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	20	0.29
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	2	0.29
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	16	0.29
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	5	0.29
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	5	0.29
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	5	0.29
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	3	0.29
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	3	0.29
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	3	0.29
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	3	0.29
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	3	0.29
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	3	0.29
(1,2721)	1:116:A:LYS:HA	1:117:A:ALA:H	9	0.29
(1,2697)	1:112:A:GLN:HG3	1:114:A:LEU:H	7	0.29
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	8	0.29
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	8	0.29
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	8	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	5	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	5	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	5	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	19	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	19	0.29
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	19	0.29
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	2	0.29
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	14	0.29
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	15	0.29
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	15	0.29
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	11	0.29
(1,1604)	1:85:A:MET:HB3	1:88:A:VAL:HG11	13	0.29
(1,1604)	1:85:A:MET:HB3	1:88:A:VAL:HG12	13	0.29
(1,1604)	1:85:A:MET:HB3	1:88:A:VAL:HG13	13	0.29
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	12	0.29
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	12	0.29
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	12	0.29
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	12	0.29
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	12	0.29
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	12	0.29
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	12	0.29
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	12	0.29
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	12	0.29
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	17	0.29
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG2	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1071)	1:115:A:GLN:H	1:115:A:GLN:HG3	12	0.29
(1,760)	1:60:A:VAL:HG11	1:67:A:GLU:HG2	12	0.29
(1,760)	1:60:A:VAL:HG12	1:67:A:GLU:HG2	12	0.29
(1,760)	1:60:A:VAL:HG13	1:67:A:GLU:HG2	12	0.29
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	2	0.29
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	7	0.29
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	20	0.29
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	18	0.29
(1,421)	1:41:A:PRO:HB3	1:42:A:SER:H	19	0.29
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	9	0.29
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	9	0.29
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	9	0.29
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	18	0.29
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	18	0.29
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	18	0.29
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	14	0.29
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	15	0.29
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	20	0.29
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	20	0.29
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	20	0.29
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD11	12	0.29
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD12	12	0.29
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD13	12	0.29
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	1	0.28
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	15	0.28
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	17	0.28
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	20	0.28
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	9	0.28
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	9	0.28
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	9	0.28
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	19	0.28
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	11	0.28
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	6	0.28
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	15	0.28
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	14	0.28
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	19	0.28
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	2	0.28
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	2	0.28
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	8	0.28
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	8	0.28
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	5	0.28
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	5	0.28
(1,3097)	1:61:A:SER:HB3	1:62:A:GLU:HB2	13	0.28
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	16	0.28
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	3	0.28
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	20	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	11	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	11	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	11	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	12	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	12	0.28
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	12	0.28
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	10	0.28
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	10	0.28
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	10	0.28
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	16	0.28
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	17	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	9	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	9	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	9	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	10	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	10	0.28
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	10	0.28
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	5	0.28
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	5	0.28
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	5	0.28
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	8	0.28
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	8	0.28
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	8	0.28
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	8	0.28
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	13	0.28
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	13	0.28
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	13	0.28
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	13	0.28
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	13	0.28
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	13	0.28
(1,2717)	1:116:A:LYS:H	1:116:A:LYS:HB3	14	0.28
(1,2571)	1:99:A:LYS:H	1:99:A:LYS:HB3	5	0.28
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	4	0.28
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	12	0.28
(1,2129)	1:53:A:LYS:H	1:54:A:GLY:HA3	16	0.28
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	6	0.28
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	5	0.28
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	5	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	8	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	8	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	8	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	8	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	8	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	8	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	12	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	12	0.28
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	12	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	12	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	12	0.28
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	12	0.28
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	3	0.28
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	3	0.28
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	20	0.28
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	20	0.28
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	20	0.28
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	20	0.28
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	20	0.28
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	20	0.28
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	13	0.28
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	13	0.28
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	13	0.28
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	10	0.28
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	13	0.28
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	11	0.28
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	7	0.28
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	7	0.28
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	7	0.28
(1,323)	1:32:A:SER:HB3	1:59:A:ARG:HB3	18	0.28
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	20	0.28
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	5	0.28
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	5	0.28
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	5	0.28
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	3	0.28
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	1	0.28
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	6	0.28
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	6	0.28
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	6	0.28
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	6	0.28
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	6	0.28
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	10	0.28
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	13	0.27
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	6	0.27
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	7	0.27
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	15	0.27
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	4	0.27
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	4	0.27
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	4	0.27
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	11	0.27
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	20	0.27
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	12	0.27
(1,3102)	1:46:A:PHE:HB2	1:47:A:SER:HB2	3	0.27
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	13	0.27
(1,3037)	1:35:A:GLY:H	1:39:A:GLN:HG3	5	0.27
(1,3023)	1:80:A:VAL:H	1:80:A:VAL:HB	11	0.27
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	3	0.27
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	15	0.27
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	6	0.27
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	6	0.27
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	8	0.27
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	8	0.27
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	8	0.27
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	12	0.27
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	4	0.27
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	4	0.27
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	4	0.27
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	4	0.27
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	4	0.27
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	4	0.27
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	6	0.27
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	6	0.27
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	6	0.27
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	12	0.27
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	1	0.27
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	11	0.27
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	7	0.27
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	7	0.27
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	7	0.27
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	12	0.27
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	4	0.27
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	19	0.27
(1,1738)	1:13:A:VAL:HG11	1:14:A:GLN:H	5	0.27
(1,1738)	1:13:A:VAL:HG12	1:14:A:GLN:H	5	0.27
(1,1738)	1:13:A:VAL:HG13	1:14:A:GLN:H	5	0.27
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	10	0.27
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	10	0.27
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	17	0.27
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	17	0.27
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	18	0.27
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	18	0.27
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	17	0.27
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	17	0.27
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	14	0.27
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	10	0.27
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	10	0.27
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	10	0.27
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB2	7	0.27
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB3	7	0.27
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	14	0.27
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	14	0.27
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	15	0.27
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	15	0.27
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	4	0.27
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	16	0.27
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	20	0.27
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	19	0.27
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	19	0.27
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	19	0.27
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	8	0.27
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	8	0.27
(1,153)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.27
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	9	0.27
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	18	0.27
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	10	0.26
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	15	0.26
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	18	0.26
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	12	0.26
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	11	0.26
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	7	0.26
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	16	0.26
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	4	0.26
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	9	0.26
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	5	0.26
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	1	0.26
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	1	0.26
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	1	0.26
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	20	0.26
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	20	0.26
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	20	0.26
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	18	0.26
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	16	0.26
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	8	0.26
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	8	0.26
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	8	0.26
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	8	0.26
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	8	0.26
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	8	0.26
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	8	0.26
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	8	0.26
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	8	0.26
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	2	0.26
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	17	0.26
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	8	0.26
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	9	0.26
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	9	0.26
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	7	0.26
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	7	0.26
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	7	0.26
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	7	0.26
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	7	0.26
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	7	0.26
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	19	0.26
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	19	0.26
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	19	0.26
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	10	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	15	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	15	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	15	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	19	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	19	0.26
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	19	0.26
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	7	0.26
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	7	0.26
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	7	0.26
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	7	0.26
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	7	0.26
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	9	0.26
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	9	0.26
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	9	0.26
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	2	0.26
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	8	0.26
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	14	0.26
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	14	0.26
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	14	0.26
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	14	0.26
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	14	0.26
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	14	0.26
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	13	0.26
(1,2697)	1:112:A:GLN:HG3	1:114:A:LEU:H	14	0.26
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	11	0.26
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	11	0.26
(1,2576)	1:98:A:THR:HA	1:100:A:ARG:H	14	0.26
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	6	0.26
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	6	0.26
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	6	0.26
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	16	0.26
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	16	0.26
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	16	0.26
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	20	0.26
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	20	0.26
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	20	0.26
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	8	0.26
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	12	0.26
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	12	0.26
(1,1884)	1:29:A:LEU:HG	1:31:A:PHE:H	6	0.26
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	4	0.26
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	9	0.26
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	2	0.26
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	2	0.26
(1,1592)	1:85:A:MET:HE1	1:96:A:ARG:HB3	18	0.26
(1,1592)	1:85:A:MET:HE2	1:96:A:ARG:HB3	18	0.26
(1,1592)	1:85:A:MET:HE3	1:96:A:ARG:HB3	18	0.26
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	19	0.26
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	19	0.26
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	19	0.26
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	19	0.26
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	19	0.26
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	19	0.26
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	19	0.26
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	19	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	3	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	3	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	3	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	3	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	3	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	3	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	6	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	6	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	6	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	6	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	6	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	6	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	10	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	10	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	10	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	10	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	10	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	10	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	15	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	15	0.26
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	15	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	15	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	15	0.26
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	15	0.26
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	10	0.26
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	15	0.26
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	11	0.26
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	11	0.26
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	11	0.26
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	11	0.26
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	11	0.26
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	11	0.26
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	18	0.26
(1,1375)	1:3:A:TYR:HE1	1:5:A:PRO:HD2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1375)	1:3:A:TYR:HE2	1:5:A:PRO:HD2	15	0.26
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	10	0.26
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	10	0.26
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	1	0.26
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	4	0.26
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	18	0.26
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	17	0.26
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	19	0.26
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	3	0.25
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	7	0.25
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	14	0.25
(2,59)	1:32:A:SER:N	1:58:A:THR:O	18	0.25
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	13	0.25
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	1	0.25
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	13	0.25
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	20	0.25
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	11	0.25
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	9	0.25
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	10	0.25
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	13	0.25
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	1	0.25
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	1	0.25
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	17	0.25
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	17	0.25
(1,3100)	1:78:A:MET:HE1	1:108:A:LEU:HG	4	0.25
(1,3100)	1:78:A:MET:HE2	1:108:A:LEU:HG	4	0.25
(1,3100)	1:78:A:MET:HE3	1:108:A:LEU:HG	4	0.25
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	14	0.25
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	14	0.25
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	14	0.25
(1,3067)	1:52:A:ASP:HB3	1:54:A:GLY:HA2	14	0.25
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	8	0.25
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	20	0.25
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	20	0.25
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	20	0.25
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	7	0.25
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	7	0.25
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	7	0.25
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	17	0.25
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	17	0.25
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	19	0.25
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	19	0.25
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	19	0.25
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	15	0.25
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	15	0.25
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	15	0.25
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	15	0.25
(1,2955)	1:13:A:VAL:HG21	1:111:A:ARG:H	19	0.25
(1,2955)	1:13:A:VAL:HG22	1:111:A:ARG:H	19	0.25
(1,2955)	1:13:A:VAL:HG23	1:111:A:ARG:H	19	0.25
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	17	0.25
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	17	0.25
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	17	0.25
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	17	0.25
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	17	0.25
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	17	0.25
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	3	0.25
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	3	0.25
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	3	0.25
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	12	0.25
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	12	0.25
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	12	0.25
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	13	0.25
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	13	0.25
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	13	0.25
(1,2810)	1:23:A:GLN:HE22	1:28:A:ILE:HD11	10	0.25
(1,2810)	1:23:A:GLN:HE22	1:28:A:ILE:HD12	10	0.25
(1,2810)	1:23:A:GLN:HE22	1:28:A:ILE:HD13	10	0.25
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	4	0.25
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	4	0.25
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	4	0.25
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	7	0.25
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	7	0.25
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	7	0.25
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	14	0.25
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	14	0.25
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	14	0.25
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	11	0.25
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	11	0.25
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	5	0.25
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	20	0.25
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	3	0.25
(1,2111)	1:51:A:THR:H	1:52:A:ASP:HB3	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	14	0.25
(1,1900)	1:32:A:SER:H	1:60:A:VAL:HG21	12	0.25
(1,1900)	1:32:A:SER:H	1:60:A:VAL:HG22	12	0.25
(1,1900)	1:32:A:SER:H	1:60:A:VAL:HG23	12	0.25
(1,1665)	1:102:A:GLU:HA	1:104:A:VAL:H	6	0.25
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	19	0.25
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	19	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	1	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	1	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	1	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	1	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	1	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	1	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	9	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	9	0.25
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	9	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	9	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	9	0.25
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	9	0.25
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	16	0.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	2	0.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	2	0.25
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	2	0.25
(1,1459)	1:48:A:GLU:HB3	1:49:A:ASP:HB3	16	0.25
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	2	0.25
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	9	0.25
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	9	0.25
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	9	0.25
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	9	0.25
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	20	0.25
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	20	0.25
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	20	0.25
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	2	0.25
(1,753)	1:60:A:VAL:HG11	1:67:A:GLU:HA	7	0.25
(1,753)	1:60:A:VAL:HG12	1:67:A:GLU:HA	7	0.25
(1,753)	1:60:A:VAL:HG13	1:67:A:GLU:HA	7	0.25
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	6	0.25
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	6	0.25
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	6	0.25
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	6	0.25
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG21	7	0.25
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG22	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG23	7	0.25
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	10	0.25
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	5	0.25
(1,424)	1:40:A:ASP:HB2	1:41:A:PRO:HD2	15	0.25
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	16	0.25
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	1	0.25
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	2	0.24
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	6	0.24
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	10	0.24
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	9	0.24
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	9	0.24
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	9	0.24
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	1	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	14	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	14	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	14	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	15	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	15	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	15	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	18	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	18	0.24
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	18	0.24
(1,3182)	1:9:A:VAL:HB	1:11:A:ALA:H	12	0.24
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	4	0.24
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	14	0.24
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	14	0.24
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	14	0.24
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	14	0.24
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	14	0.24
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	14	0.24
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	14	0.24
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	14	0.24
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	14	0.24
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	3	0.24
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	7	0.24
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	9	0.24
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	4	0.24
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	6	0.24
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	6	0.24
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	6	0.24
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	19	0.24
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	15	0.24
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	11	0.24
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	11	0.24
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	16	0.24
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	16	0.24
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	4	0.24
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	17	0.24
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	17	0.24
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	17	0.24
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	1	0.24
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	17	0.24
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	19	0.24
(1,2987)	1:4:A:ILE:H	1:8:A:PRO:HD3	12	0.24
(1,2980)	1:14:A:GLN:HE22	1:109:A:VAL:H	19	0.24
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	11	0.24
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	7	0.24
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	7	0.24
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	6	0.24
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	6	0.24
(1,2842)	1:72:A:GLN:HE22	1:111:A:ARG:HG3	20	0.24
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG21	7	0.24
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG22	7	0.24
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG23	7	0.24
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	8	0.24
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	18	0.24
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	17	0.24
(1,2566)	1:97:A:LEU:HD11	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD12	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD13	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD21	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD22	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD23	1:99:A:LYS:H	8	0.24
(1,2566)	1:97:A:LEU:HD11	1:99:A:LYS:H	17	0.24
(1,2566)	1:97:A:LEU:HD12	1:99:A:LYS:H	17	0.24
(1,2566)	1:97:A:LEU:HD13	1:99:A:LYS:H	17	0.24
(1,2566)	1:97:A:LEU:HD21	1:99:A:LYS:H	17	0.24
(1,2566)	1:97:A:LEU:HD22	1:99:A:LYS:H	17	0.24
(1,2566)	1:97:A:LEU:HD23	1:99:A:LYS:H	17	0.24
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	15	0.24
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	15	0.24
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	15	0.24
(1,2454)	1:37:A:ILE:HG13	1:90:A:HIS:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	14	0.24
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	12	0.24
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	19	0.24
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	2	0.24
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	2	0.24
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	11	0.24
(1,2083)	1:47:A:SER:HB2	1:49:A:ASP:H	6	0.24
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	14	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	16	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	16	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	16	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	16	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	16	0.24
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	16	0.24
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	8	0.24
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	13	0.24
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	3	0.24
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE2	10	0.24
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE3	10	0.24
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	8	0.24
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	8	0.24
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	8	0.24
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	12	0.24
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	12	0.24
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	12	0.24
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	12	0.24
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	12	0.24
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	12	0.24
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	6	0.24
(1,1311)	1:88:A:VAL:HG11	1:92:A:GLN:HB2	13	0.24
(1,1311)	1:88:A:VAL:HG12	1:92:A:GLN:HB2	13	0.24
(1,1311)	1:88:A:VAL:HG13	1:92:A:GLN:HB2	13	0.24
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	4	0.24
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	4	0.24
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	4	0.24
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	11	0.24
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	17	0.24
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	17	0.24
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	17	0.24
(1,843)	1:95:A:LYS:HA	1:95:A:LYS:HG2	9	0.24
(1,843)	1:95:A:LYS:HA	1:95:A:LYS:HG2	18	0.24
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	17	0.24
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	7	0.24
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	5	0.24
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	11	0.24
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	4	0.24
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	4	0.24
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	4	0.24
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	15	0.24
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	15	0.24
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	15	0.24
(1,153)	1:14:A:GLN:H	1:14:A:GLN:HG3	15	0.24
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	6	0.24
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	15	0.24
(1,56)	1:4:A:ILE:HG21	1:5:A:PRO:HD3	13	0.24
(1,56)	1:4:A:ILE:HG22	1:5:A:PRO:HD3	13	0.24
(1,56)	1:4:A:ILE:HG23	1:5:A:PRO:HD3	13	0.24
(1,14)	1:15:A:ARG:HD2	1:16:A:VAL:HA	4	0.24
(1,14)	1:15:A:ARG:HD3	1:16:A:VAL:HA	4	0.24
(2,58)	1:59:A:ARG:O	1:73:A:ILE:H	7	0.23
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	3	0.23
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	10	0.23
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	16	0.23
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	20	0.23
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	17	0.23
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	17	0.23
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	17	0.23
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	16	0.23
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	14	0.23
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	14	0.23
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	14	0.23
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	5	0.23
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	5	0.23
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	5	0.23
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	12	0.23
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	1	0.23
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	10	0.23
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	18	0.23
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	18	0.23
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	1	0.23
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	1	0.23
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	1	0.23
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	15	0.23
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	15	0.23
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	18	0.23
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	20	0.23
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	20	0.23
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	20	0.23
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	2	0.23
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	13	0.23
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	13	0.23
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	8	0.23
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	17	0.23
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	2	0.23
(1,2987)	1:4:A:ILE:H	1:8:A:PRO:HD3	11	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	1	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	1	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	1	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	6	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	6	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	6	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	16	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	16	0.23
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	16	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	9	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	9	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	9	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	9	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	9	0.23
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	9	0.23
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	17	0.23
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG21	9	0.23
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG22	9	0.23
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG23	9	0.23
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	4	0.23
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	4	0.23
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	10	0.23
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	10	0.23
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	16	0.23
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	2	0.23
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	3	0.23
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	5	0.23
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	13	0.23
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	14	0.23
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	14	0.23
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	12	0.23
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	6	0.23
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	10	0.23
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	10	0.23
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	3	0.23
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	3	0.23
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	10	0.23
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	10	0.23
(1,1615)	1:56:A:TYR:HD1	1:57:A:VAL:HA	16	0.23
(1,1615)	1:56:A:TYR:HD2	1:57:A:VAL:HA	16	0.23
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	18	0.23
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	9	0.23
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	9	0.23
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	9	0.23
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	9	0.23
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	9	0.23
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	9	0.23
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	9	0.23
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	9	0.23
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	9	0.23
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	2	0.23
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	2	0.23
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	2	0.23
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	2	0.23
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	2	0.23
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	2	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	8	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	8	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	8	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	8	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	8	0.23
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	8	0.23
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	8	0.23
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	18	0.23
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:14:A:GLN:H	1:111:A:ARG:HB2	14	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	8	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	8	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	8	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	8	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	8	0.23
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	8	0.23
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	8	0.23
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	3	0.23
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	3	0.23
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	3	0.23
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	3	0.23
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	3	0.23
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	3	0.23
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	17	0.23
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	17	0.23
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	17	0.23
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	5	0.23
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	5	0.23
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	5	0.23
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	1	0.23
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	1	0.23
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	1	0.23
(1,843)	1:95:A:LYS:HA	1:95:A:LYS:HG2	7	0.23
(1,753)	1:60:A:VAL:HG11	1:67:A:GLU:HA	12	0.23
(1,753)	1:60:A:VAL:HG12	1:67:A:GLU:HA	12	0.23
(1,753)	1:60:A:VAL:HG13	1:67:A:GLU:HA	12	0.23
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	19	0.23
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	4	0.23
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	15	0.23
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	5	0.23
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	5	0.23
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	5	0.23
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	9	0.23
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	9	0.23
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	9	0.23
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG21	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG22	12	0.23
(1,652)	1:60:A:VAL:H	1:60:A:VAL:HG23	12	0.23
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	15	0.23
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	1	0.23
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	1	0.23
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	1	0.23
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	2	0.23
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	2	0.23
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	2	0.23
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	3	0.23
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	3	0.23
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	3	0.23
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	15	0.23
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	15	0.23
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	15	0.23
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	10	0.23
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	10	0.23
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	10	0.23
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	2	0.23
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	14	0.23
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	14	0.23
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	14	0.23
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG21	17	0.23
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG22	17	0.23
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG23	17	0.23
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG21	17	0.23
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG22	17	0.23
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG23	17	0.23
(1,5)	1:49:A:ASP:HB2	1:51:A:THR:HA	7	0.23
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	8	0.22
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	9	0.22
(2,59)	1:32:A:SER:N	1:58:A:THR:O	14	0.22
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	1	0.22
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	9	0.22
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	11	0.22
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	3	0.22
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	11	0.22
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	13	0.22
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	18	0.22
(1,3192)	1:33:A:ILE:HG21	1:59:A:ARG:H	6	0.22
(1,3192)	1:33:A:ILE:HG22	1:59:A:ARG:H	6	0.22
(1,3192)	1:33:A:ILE:HG23	1:59:A:ARG:H	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	14	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	2	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	2	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	2	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	13	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	13	0.22
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	13	0.22
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	14	0.22
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	8	0.22
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	8	0.22
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	8	0.22
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	8	0.22
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	8	0.22
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	8	0.22
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	18	0.22
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	7	0.22
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	8	0.22
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	9	0.22
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	17	0.22
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	18	0.22
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	19	0.22
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	16	0.22
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	5	0.22
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	5	0.22
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	5	0.22
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	6	0.22
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	6	0.22
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	6	0.22
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	6	0.22
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	10	0.22
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	10	0.22
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	10	0.22
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	3	0.22
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	3	0.22
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	3	0.22
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	19	0.22
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	19	0.22
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	6	0.22
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	9	0.22
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	3	0.22
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	3	0.22
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	3	0.22
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD2	5	0.22
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD3	5	0.22
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	18	0.22
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	18	0.22
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	18	0.22
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	18	0.22
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	1	0.22
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	1	0.22
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	1	0.22
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	1	0.22
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	1	0.22
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	1	0.22
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	1	0.22
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	7	0.22
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	9	0.22
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	13	0.22
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	9	0.22
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	18	0.22
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	18	0.22
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	18	0.22
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	19	0.22
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	19	0.22
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	19	0.22
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	13	0.22
(1,2576)	1:98:A:THR:HA	1:100:A:ARG:H	12	0.22
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	2	0.22
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	2	0.22
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	2	0.22
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	20	0.22
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	10	0.22
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	15	0.22
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	15	0.22
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	15	0.22
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	20	0.22
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	20	0.22
(1,2111)	1:51:A:THR:H	1:52:A:ASP:HB3	2	0.22
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	18	0.22
(1,2012)	1:40:A:ASP:H	1:41:A:PRO:HD2	3	0.22
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	17	0.22
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	5	0.22
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	19	0.22
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	19	0.22
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	19	0.22
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	7	0.22
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	7	0.22
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	3	0.22
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	3	0.22
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	3	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	4	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	4	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	4	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	4	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	4	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	4	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	4	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	4	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	4	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	18	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	18	0.22
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	18	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	18	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	18	0.22
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	18	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	18	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	18	0.22
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	18	0.22
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	4	0.22
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	4	0.22
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	4	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	4	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	4	0.22
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	4	0.22
(1,1536)	1:13:A:VAL:HA	1:110:A:THR:HA	19	0.22
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	2	0.22
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	6	0.22
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	17	0.22
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	17	0.22
(1,1375)	1:3:A:TYR:HE1	1:5:A:PRO:HD2	17	0.22
(1,1375)	1:3:A:TYR:HE2	1:5:A:PRO:HD2	17	0.22
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	6	0.22
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	6	0.22
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	20	0.22
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	20	0.22
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	20	0.22
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	7	0.22
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	7	0.22
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	7	0.22
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	5	0.22
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	5	0.22
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	3	0.22
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	6	0.22
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	8	0.22
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	12	0.22
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	12	0.22
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	11	0.22
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	8	0.22
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	7	0.22
(1,411)	1:39:A:GLN:HG2	1:90:A:HIS:HB3	19	0.22
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	2	0.22
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	4	0.22
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	18	0.22
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	15	0.22
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	15	0.22
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	15	0.22
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	6	0.22
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	6	0.22
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	6	0.22
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	17	0.22
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	9	0.22
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	9	0.22
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	9	0.22
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	10	0.22
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	12	0.22
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	11	0.21
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	16	0.21
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	14	0.21
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	16	0.21
(2,55)	1:55:A:ILE:H	1:77:A:ILE:O	20	0.21
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	8	0.21
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	12	0.21
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	14	0.21
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	19	0.21
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	4	0.21
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	2	0.21
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	14	0.21
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	6	0.21
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	11	0.21
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	11	0.21
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	11	0.21
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	6	0.21
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	10	0.21
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	17	0.21
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	1	0.21
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	14	0.21
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	16	0.21
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	20	0.21
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	11	0.21
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	20	0.21
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	13	0.21
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	17	0.21
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	3	0.21
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	3	0.21
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	3	0.21
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	8	0.21
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	8	0.21
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	8	0.21
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	10	0.21
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	10	0.21
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	10	0.21
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	13	0.21
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	13	0.21
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	13	0.21
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	7	0.21
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	7	0.21
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	7	0.21
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	14	0.21
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	11	0.21
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	3	0.21
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	14	0.21
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	5	0.21
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	7	0.21
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	12	0.21
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	20	0.21
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	10	0.21
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	10	0.21
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	11	0.21
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	11	0.21
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	11	0.21
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	3	0.21
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	3	0.21
(1,2915)	1:79:A:GLN:HE22	1:84:A:ASP:H	18	0.21
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	5	0.21
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	4	0.21
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	17	0.21
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	17	0.21
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	17	0.21
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	20	0.21
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	19	0.21
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	19	0.21
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	7	0.21
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	14	0.21
(1,2717)	1:116:A:LYS:H	1:116:A:LYS:HB3	13	0.21
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	5	0.21
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	5	0.21
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	5	0.21
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	2	0.21
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	3	0.21
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	3	0.21
(1,2424)	1:85:A:MET:HG3	1:86:A:THR:H	15	0.21
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	3	0.21
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	3	0.21
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	16	0.21
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	17	0.21
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	20	0.21
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	18	0.21
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	8	0.21
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	12	0.21
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	3	0.21
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	6	0.21
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	6	0.21
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	18	0.21
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	18	0.21
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	18	0.21
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	1	0.21
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	1	0.21
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	10	0.21
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	10	0.21
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	10	0.21
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	12	0.21
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	12	0.21
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	14	0.21
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	14	0.21
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	10	0.21
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	10	0.21
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	15	0.21
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	17	0.21
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	17	0.21
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	17	0.21
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	17	0.21
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	17	0.21
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	12	0.21
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	20	0.21
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	17	0.21
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	17	0.21
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	17	0.21
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	17	0.21
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	17	0.21
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	17	0.21
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	11	0.21
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	11	0.21
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	14	0.21
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	14	0.21
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	14	0.21
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	18	0.21
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	18	0.21
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	18	0.21
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	12	0.21
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	12	0.21
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	12	0.21
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB2	14	0.21
(1,1062)	1:112:A:GLN:HG3	1:113:A:SER:HB3	14	0.21
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	8	0.21
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	8	0.21
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	18	0.21
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	18	0.21
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	11	0.21
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	11	0.21
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	11	0.21
(1,981)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	12	0.21
(1,981)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	12	0.21
(1,981)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	12	0.21
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	3	0.21
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	20	0.21
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	6	0.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	2	0.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	2	0.21
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	2	0.21
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	5	0.21
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	16	0.21
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	13	0.21
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	9	0.21
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	9	0.21
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	9	0.21
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	1	0.21
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	1	0.21
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	1	0.21
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	1	0.21
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	1	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	14	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	14	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	14	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	15	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	15	0.21
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	15	0.21
(1,16)	1:49:A:ASP:HB2	1:51:A:THR:HA	7	0.21
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	17	0.2
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	12	0.2
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	18	0.2
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	15	0.2
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	16	0.2
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	8	0.2
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	11	0.2
(1,3191)	1:48:A:GLU:HB2	1:52:A:ASP:H	17	0.2
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	7	0.2
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	15	0.2
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	15	0.2
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	15	0.2
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	18	0.2
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	4	0.2
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	16	0.2
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	6	0.2
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	13	0.2
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	10	0.2
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	1	0.2
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	13	0.2
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	14	0.2
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	17	0.2
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	1	0.2
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	1	0.2
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	1	0.2
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	9	0.2
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	9	0.2
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	9	0.2
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	11	0.2
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	11	0.2
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	11	0.2
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	9	0.2
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	12	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	5	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	5	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	5	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	16	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	16	0.2
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	16	0.2
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	13	0.2
(1,3019)	1:19:A:HIS:HB2	1:105:A:VAL:H	20	0.2
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	3	0.2
(1,3012)	1:36:A:GLY:HA2	1:92:A:GLN:H	8	0.2
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	5	0.2
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	5	0.2
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	18	0.2
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	8	0.2
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	9	0.2
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	15	0.2
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	15	0.2
(1,2980)	1:14:A:GLN:HE22	1:109:A:VAL:H	6	0.2
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	19	0.2
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	2	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	2	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	2	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	13	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	13	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	13	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	17	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	17	0.2
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	17	0.2
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	6	0.2
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	6	0.2
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	6	0.2
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	6	0.2
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	6	0.2
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	6	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	4	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	13	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	13	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	13	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	13	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	13	0.2
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	13	0.2
(1,2852)	1:56:A:TYR:HD1	1:75:A:ASP:H	7	0.2
(1,2852)	1:56:A:TYR:HD2	1:75:A:ASP:H	7	0.2
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	6	0.2
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	6	0.2
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	6	0.2
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	6	0.2
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB2	5	0.2
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB3	5	0.2
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	3	0.2
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	7	0.2
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	12	0.2
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	14	0.2
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	14	0.2
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	17	0.2
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD21	16	0.2
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD22	16	0.2
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD23	16	0.2
(1,2578)	1:99:A:LYS:HG2	1:100:A:ARG:H	16	0.2
(1,2574)	1:99:A:LYS:H	1:100:A:ARG:HA	5	0.2
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	1	0.2
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	1	0.2
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	1	0.2
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	1	0.2
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	1	0.2
(1,2411)	1:84:A:ASP:H	1:84:A:ASP:HB2	11	0.2
(1,2411)	1:84:A:ASP:H	1:84:A:ASP:HB2	16	0.2
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	16	0.2
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	20	0.2
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	1	0.2
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	1	0.2
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	4	0.2
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	4	0.2
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	6	0.2
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	6	0.2
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	9	0.2
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	9	0.2
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	18	0.2
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	8	0.2
(1,2111)	1:51:A:THR:H	1:52:A:ASP:HB3	11	0.2
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	10	0.2
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	15	0.2
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	3	0.2
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	2	0.2
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	11	0.2
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	20	0.2
(1,1678)	1:118:A:VAL:H	1:120:A:GLN:HE22	6	0.2
(1,1662)	1:113:A:SER:HB2	1:114:A:LEU:H	14	0.2
(1,1662)	1:113:A:SER:HB3	1:114:A:LEU:H	14	0.2
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	8	0.2
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	8	0.2
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	11	0.2
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	11	0.2
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	7	0.2
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	7	0.2
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	7	0.2
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	1	0.2
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	8	0.2
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	8	0.2
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	16	0.2
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	16	0.2
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	18	0.2
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	18	0.2
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	18	0.2
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	18	0.2
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	18	0.2
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	18	0.2
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	2	0.2
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	2	0.2
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	2	0.2
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	3	0.2
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	18	0.2
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	18	0.2
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	18	0.2
(1,1458)	1:23:A:GLN:HB2	1:26:A:ASN:HB2	1	0.2
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD11	7	0.2
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD12	7	0.2
(1,1453)	1:23:A:GLN:HB3	1:28:A:ILE:HD13	7	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	6	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	6	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	6	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	18	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	18	0.2
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	18	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	12	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	12	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	12	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	19	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	19	0.2
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	19	0.2
(1,1408)	1:34:A:GLY:HA3	1:90:A:HIS:HE1	19	0.2
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	9	0.2
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	9	0.2
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	9	0.2
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	8	0.2
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	8	0.2
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	8	0.2
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	17	0.2
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	17	0.2
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	17	0.2
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	2	0.2
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	2	0.2
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	2	0.2
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	16	0.2
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	16	0.2
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	16	0.2
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	17	0.2
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	1	0.2
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	1	0.2
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	11	0.2
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	11	0.2
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	2	0.2
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	2	0.2
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	6	0.2
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	6	0.2
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	6	0.2
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	18	0.2
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	18	0.2
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	18	0.2
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	2	0.2
(1,684)	1:62:A:GLU:HB3	1:63:A:GLY:HA2	9	0.2
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	14	0.2
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	7	0.2
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	13	0.2
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	3	0.2
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	5	0.2
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	5	0.2
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	5	0.2
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	18	0.2
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	18	0.2
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	18	0.2
(1,117)	1:10:A:THR:HB	1:11:A:ALA:H	4	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	1	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	1	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	1	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	8	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	8	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	8	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	18	0.2
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	18	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG21	2	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG22	2	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG23	2	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG21	2	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG22	2	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG23	2	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG21	20	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG22	20	0.2
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG23	20	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG21	20	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG22	20	0.2
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG23	20	0.2
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	6	0.19
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	2	0.19
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	4	0.19
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	7	0.19
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	11	0.19
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	10	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	7	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	7	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	7	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	10	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	10	0.19
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	10	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	13	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	13	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	13	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	18	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	18	0.19
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	18	0.19
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	8	0.19
(1,3156)	1:36:A:GLY:H	1:55:A:ILE:H	19	0.19
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	7	0.19
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	18	0.19
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	3	0.19
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	4	0.19
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	6	0.19
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	9	0.19
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	3	0.19
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	17	0.19
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	19	0.19
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	2	0.19
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	2	0.19
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	2	0.19
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	4	0.19
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	4	0.19
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	4	0.19
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	20	0.19
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	20	0.19
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	20	0.19
(1,3051)	1:29:A:LEU:HA	1:65:A:PRO:HG3	9	0.19
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	3	0.19
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	2	0.19
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	3	0.19
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	12	0.19
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	16	0.19
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	10	0.19
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	10	0.19
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	10	0.19
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	14	0.19
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	14	0.19
(1,3002)	1:56:A:TYR:H	1:57:A:VAL:HB	1	0.19
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	17	0.19
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	17	0.19
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	14	0.19
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	6	0.19
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	11	0.19
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	14	0.19
(1,2986)	1:72:A:GLN:HE22	1:113:A:SER:H	7	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	4	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	4	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	4	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	8	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	8	0.19
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	8	0.19
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	20	0.19
(1,2846)	1:57:A:VAL:HB	1:74:A:GLY:H	15	0.19
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	17	0.19
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	10	0.19
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	13	0.19
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	11	0.19
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	11	0.19
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	16	0.19
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	16	0.19
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	18	0.19
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	18	0.19
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	9	0.19
(1,2722)	1:116:A:LYS:HB2	1:117:A:ALA:H	4	0.19
(1,2689)	1:111:A:ARG:HG3	1:113:A:SER:H	20	0.19
(1,2681)	1:110:A:THR:HB	1:112:A:GLN:HE21	18	0.19
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	13	0.19
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	13	0.19
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	11	0.19
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	11	0.19
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	11	0.19
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	13	0.19
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	13	0.19
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	13	0.19
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	5	0.19
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	5	0.19
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	8	0.19
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	8	0.19
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	19	0.19
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	19	0.19
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	14	0.19
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	13	0.19
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	13	0.19
(1,2039)	1:43:A:GLN:HB3	1:43:A:GLN:HE21	2	0.19
(1,2039)	1:43:A:GLN:HB3	1:43:A:GLN:HE21	20	0.19
(1,2018)	1:41:A:PRO:HB3	1:42:A:SER:H	19	0.19
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	5	0.19
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	15	0.19
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	15	0.19
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	16	0.19
(1,1662)	1:113:A:SER:HB2	1:114:A:LEU:H	7	0.19
(1,1662)	1:113:A:SER:HB3	1:114:A:LEU:H	7	0.19
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	17	0.19
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	17	0.19
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	18	0.19
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	13	0.19
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	13	0.19
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	6	0.19
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	6	0.19
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	8	0.19
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	15	0.19
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	15	0.19
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	15	0.19
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	15	0.19
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	15	0.19
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	15	0.19
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	15	0.19
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	15	0.19
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	15	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	16	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	16	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	16	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	16	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	16	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	16	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	20	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	20	0.19
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	20	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	20	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	20	0.19
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	20	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	18	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	18	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	18	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	18	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	18	0.19
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	18	0.19
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	18	0.19
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	3	0.19
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	3	0.19
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	3	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	4	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	4	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	4	0.19
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	4	0.19
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	4	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	18	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	18	0.19
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	18	0.19
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	18	0.19
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	18	0.19
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	18	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	2	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	2	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	2	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	17	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	17	0.19
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	17	0.19
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	19	0.19
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	19	0.19
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	19	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	18	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	18	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	18	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	18	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	18	0.19
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	18	0.19
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	18	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	2	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	2	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	2	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	17	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	17	0.19
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	17	0.19
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	3	0.19
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	3	0.19
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	3	0.19
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	15	0.19
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	15	0.19
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	19	0.19
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	19	0.19
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	19	0.19
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	16	0.19
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	16	0.19
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	16	0.19
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	15	0.19
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	15	0.19
(1,1067)	1:115:A:GLN:HA	1:115:A:GLN:HE21	17	0.19
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	18	0.19
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	18	0.19
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	18	0.19
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	18	0.19
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	18	0.19
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	18	0.19
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	6	0.19
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	6	0.19
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	6	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	5	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	5	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	5	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	13	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	13	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	13	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	19	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	19	0.19
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	19	0.19
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	7	0.19
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	10	0.19
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	10	0.19
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	10	0.19
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	1	0.19
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	12	0.19
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	17	0.19
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	19	0.19
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	14	0.19
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	15	0.19
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	18	0.19
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	15	0.19
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	4	0.19
(1,424)	1:40:A:ASP:HB2	1:41:A:PRO:HD2	19	0.19
(1,411)	1:39:A:GLN:HG2	1:90:A:HIS:HB3	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	1	0.19
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	11	0.19
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	17	0.19
(1,359)	1:36:A:GLY:HA3	1:37:A:ILE:HG13	3	0.19
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	7	0.19
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	7	0.19
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	7	0.19
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	20	0.19
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	1	0.19
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	10	0.19
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	10	0.19
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	5	0.19
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	5	0.19
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	5	0.19
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	19	0.19
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	14	0.19
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	14	0.19
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	14	0.19
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	15	0.19
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	15	0.19
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	15	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	9	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	9	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	9	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG21	12	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG22	12	0.19
(1,113)	1:10:A:THR:HA	1:10:A:THR:HG23	12	0.19
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	5	0.18
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	5	0.18
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	17	0.18
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	10	0.18
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	17	0.18
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	18	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	3	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	3	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	3	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	8	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	8	0.18
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	8	0.18
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	2	0.18
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	2	0.18
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	14	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	15	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	15	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	15	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	15	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	15	0.18
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	15	0.18
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	15	0.18
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	15	0.18
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	20	0.18
(1,3138)	1:14:A:GLN:H	1:111:A:ARG:HD2	9	0.18
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	18	0.18
(1,3121)	1:72:A:GLN:HA	1:72:A:GLN:HE22	2	0.18
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	17	0.18
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	4	0.18
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	4	0.18
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	14	0.18
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	14	0.18
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	1	0.18
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	17	0.18
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	17	0.18
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	17	0.18
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	17	0.18
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	17	0.18
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	17	0.18
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	8	0.18
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	20	0.18
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	2	0.18
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	2	0.18
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	2	0.18
(1,3020)	1:82:A:GLY:H	1:108:A:LEU:H	6	0.18
(1,3019)	1:19:A:HIS:HB2	1:105:A:VAL:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3017)	1:20:A:LYS:HG2	1:101:A:SER:H	3	0.18
(1,3017)	1:20:A:LYS:HG3	1:101:A:SER:H	3	0.18
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	9	0.18
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	9	0.18
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	6	0.18
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	6	0.18
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	12	0.18
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG11	13	0.18
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG12	13	0.18
(1,2996)	1:31:A:PHE:H	1:60:A:VAL:HG13	13	0.18
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	8	0.18
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	10	0.18
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	13	0.18
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	18	0.18
(1,2987)	1:4:A:ILE:H	1:8:A:PRO:HD3	7	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	12	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	12	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	12	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	14	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	14	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	14	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	19	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	19	0.18
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	19	0.18
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	1	0.18
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG11	8	0.18
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG12	8	0.18
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG13	8	0.18
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	11	0.18
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	11	0.18
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	11	0.18
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	18	0.18
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	18	0.18
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	18	0.18
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	18	0.18
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	18	0.18
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	18	0.18
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	10	0.18
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	10	0.18
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	10	0.18
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	10	0.18
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	10	0.18
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	19	0.18
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	20	0.18
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB2	19	0.18
(1,2795)	1:21:A:LEU:H	1:27:A:LEU:HB3	19	0.18
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	3	0.18
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	2	0.18
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	12	0.18
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	9	0.18
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	9	0.18
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	9	0.18
(1,2576)	1:98:A:THR:HA	1:100:A:ARG:H	16	0.18
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	14	0.18
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	14	0.18
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	14	0.18
(1,2452)	1:36:A:GLY:HA2	1:90:A:HIS:H	12	0.18
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	13	0.18
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	13	0.18
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	14	0.18
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	17	0.18
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	17	0.18
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	10	0.18
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	18	0.18
(1,2176)	1:32:A:SER:HB2	1:59:A:ARG:H	10	0.18
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE1	5	0.18
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE2	5	0.18
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	19	0.18
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	18	0.18
(1,1857)	1:27:A:LEU:H	1:27:A:LEU:HG	4	0.18
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	11	0.18
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	16	0.18
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	19	0.18
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	20	0.18
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	3	0.18
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	3	0.18
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	5	0.18
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	20	0.18
(1,1662)	1:113:A:SER:HB2	1:114:A:LEU:H	19	0.18
(1,1662)	1:113:A:SER:HB3	1:114:A:LEU:H	19	0.18
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG2	3	0.18
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG3	3	0.18
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	7	0.18
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	7	0.18
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	7	0.18
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	7	0.18
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	11	0.18
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	11	0.18
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	6	0.18
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	6	0.18
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	13	0.18
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	13	0.18
(1,1624)	1:46:A:PHE:H	1:47:A:SER:HB2	2	0.18
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	5	0.18
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	5	0.18
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	1	0.18
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	1	0.18
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	1	0.18
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	4	0.18
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	8	0.18
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	8	0.18
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	8	0.18
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	17	0.18
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	17	0.18
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	17	0.18
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	17	0.18
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	17	0.18
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	17	0.18
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	17	0.18
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	17	0.18
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	17	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	5	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	5	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	5	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	5	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	5	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	5	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	14	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	14	0.18
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	14	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	14	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	14	0.18
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	14	0.18
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	16	0.18
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	16	0.18
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	16	0.18
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	16	0.18
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	16	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	8	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	8	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	8	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	11	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	11	0.18
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	11	0.18
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG21	9	0.18
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG22	9	0.18
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG23	9	0.18
(1,1469)	1:78:A:MET:HB2	1:108:A:LEU:HB2	20	0.18
(1,1469)	1:78:A:MET:HB2	1:108:A:LEU:HB3	20	0.18
(1,1458)	1:23:A:GLN:HB2	1:26:A:ASN:HB2	10	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	8	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	8	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	8	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	11	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	11	0.18
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	11	0.18
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	4	0.18
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	4	0.18
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	4	0.18
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	13	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	4	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	4	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	4	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	11	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	11	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	11	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	16	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	16	0.18
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	16	0.18
(1,1295)	1:91:A:ASP:H	1:91:A:ASP:HB2	12	0.18
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	14	0.18
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	14	0.18
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	14	0.18
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	14	0.18
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	18	0.18
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	18	0.18
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	15	0.18
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	15	0.18
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	15	0.18
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	12	0.18
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	12	0.18
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	12	0.18
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	6	0.18
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	8	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	2	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	2	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	2	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	10	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	10	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	10	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	14	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	14	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	14	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	20	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	20	0.18
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	20	0.18
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	2	0.18
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	5	0.18
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	8	0.18
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	10	0.18
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	13	0.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	18	0.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	18	0.18
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	18	0.18
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	9	0.18
(1,551)	1:52:A:ASP:HA	1:53:A:LYS:H	3	0.18
(1,548)	1:51:A:THR:H	1:51:A:THR:HG21	15	0.18
(1,548)	1:51:A:THR:H	1:51:A:THR:HG22	15	0.18
(1,548)	1:51:A:THR:H	1:51:A:THR:HG23	15	0.18
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	2	0.18
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	3	0.18
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	12	0.18
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	13	0.18
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	4	0.18
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	10	0.18
(1,424)	1:40:A:ASP:HB2	1:41:A:PRO:HD2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	20	0.18
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	10	0.18
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	10	0.18
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	10	0.18
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	13	0.18
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	13	0.18
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	13	0.18
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	17	0.18
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	17	0.18
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	17	0.18
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	11	0.18
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	14	0.18
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	14	0.18
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	16	0.18
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	16	0.18
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	17	0.18
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	17	0.18
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	12	0.18
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	12	0.18
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	12	0.18
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	13	0.18
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	13	0.18
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	13	0.18
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	7	0.18
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	7	0.18
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	7	0.18
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	7	0.18
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	7	0.18
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	7	0.18
(1,87)	1:8:A:PRO:HA	1:9:A:VAL:H	9	0.18
(1,55)	1:4:A:ILE:HB	1:5:A:PRO:HD3	7	0.18
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	4	0.17
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	20	0.17
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	6	0.17
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	18	0.17
(2,24)	1:57:A:VAL:O	1:75:A:ASP:H	20	0.17
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	8	0.17
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	18	0.17
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	19	0.17
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	19	0.17
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	19	0.17
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	4	0.17
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	4	0.17
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	16	0.17
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	16	0.17
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	16	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	4	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	4	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	4	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	10	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	10	0.17
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	10	0.17
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	6	0.17
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	6	0.17
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	6	0.17
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	8	0.17
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	12	0.17
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	12	0.17
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	12	0.17
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	12	0.17
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	12	0.17
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	12	0.17
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	12	0.17
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	12	0.17
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	12	0.17
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	14	0.17
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	8	0.17
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	11	0.17
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	17	0.17
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	19	0.17
(1,3123)	1:79:A:GLN:HE22	1:84:A:ASP:HB2	16	0.17
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD2	15	0.17
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD3	15	0.17
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	3	0.17
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	3	0.17
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	3	0.17
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	3	0.17
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	15	0.17
(1,3079)	1:47:A:SER:HB2	1:48:A:GLU:HB2	14	0.17
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	12	0.17
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	12	0.17
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	12	0.17
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	20	0.17
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	20	0.17
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG21	20	0.17
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG22	20	0.17
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG23	20	0.17
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	12	0.17
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	12	0.17
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	12	0.17
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	10	0.17
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	12	0.17
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	12	0.17
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	18	0.17
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	7	0.17
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	1	0.17
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	10	0.17
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	11	0.17
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	2	0.17
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	2	0.17
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	8	0.17
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	8	0.17
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	16	0.17
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	16	0.17
(1,2998)	1:37:A:ILE:HG12	1:39:A:GLN:H	5	0.17
(1,2997)	1:36:A:GLY:H	1:39:A:GLN:HA	3	0.17
(1,2981)	1:50:A:LYS:HD2	1:110:A:THR:H	15	0.17
(1,2981)	1:50:A:LYS:HD3	1:110:A:THR:H	15	0.17
(1,2979)	1:38:A:ASP:HA	1:89:A:THR:H	12	0.17
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	17	0.17
(1,2976)	1:99:A:LYS:HB2	1:101:A:SER:H	18	0.17
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD2	15	0.17
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD3	15	0.17
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	12	0.17
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	2	0.17
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	8	0.17
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	13	0.17
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	17	0.17
(1,2955)	1:13:A:VAL:HG21	1:111:A:ARG:H	11	0.17
(1,2955)	1:13:A:VAL:HG22	1:111:A:ARG:H	11	0.17
(1,2955)	1:13:A:VAL:HG23	1:111:A:ARG:H	11	0.17
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	5	0.17
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	8	0.17
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	8	0.17
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	8	0.17
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	8	0.17
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	8	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	1	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	1	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	1	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	1	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	1	0.17
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	1	0.17
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	14	0.17
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	10	0.17
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG21	14	0.17
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG22	14	0.17
(1,2778)	1:14:A:GLN:HE21	1:109:A:VAL:HG23	14	0.17
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	16	0.17
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	19	0.17
(1,2670)	1:112:A:GLN:H	1:112:A:GLN:HB2	4	0.17
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	15	0.17
(1,2564)	1:95:A:LYS:HE2	1:99:A:LYS:H	19	0.17
(1,2564)	1:95:A:LYS:HE3	1:99:A:LYS:H	19	0.17
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	15	0.17
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	12	0.17
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	18	0.17
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	18	0.17
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	8	0.17
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	6	0.17
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	6	0.17
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	9	0.17
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	9	0.17
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	1	0.17
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	5	0.17
(1,2176)	1:32:A:SER:HB2	1:59:A:ARG:H	5	0.17
(1,2043)	1:41:A:PRO:HA	1:44:A:ASN:H	11	0.17
(1,2043)	1:41:A:PRO:HA	1:44:A:ASN:H	15	0.17
(1,1989)	1:36:A:GLY:HA2	1:39:A:GLN:HE22	8	0.17
(1,1757)	1:15:A:ARG:H	1:15:A:ARG:HB3	11	0.17
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	11	0.17
(1,1712)	1:10:A:THR:H	1:10:A:THR:HB	7	0.17
(1,1677)	1:35:A:GLY:HA3	1:56:A:TYR:H	5	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD11	5	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD13	5	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD11	19	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD12	19	0.17
(1,1676)	1:35:A:GLY:H	1:55:A:ILE:HD13	19	0.17
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	8	0.17
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	1	0.17
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	1	0.17
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	1	0.17
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	17	0.17
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	17	0.17
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	17	0.17
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	16	0.17
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	9	0.17
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	9	0.17
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	9	0.17
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	20	0.17
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	20	0.17
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	20	0.17
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	9	0.17
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	9	0.17
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	9	0.17
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	11	0.17
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	11	0.17
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	7	0.17
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	7	0.17
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	7	0.17
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	3	0.17
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	17	0.17
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	1	0.17
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	1	0.17
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	1	0.17
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	1	0.17
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	1	0.17
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	1	0.17
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	1	0.17
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	1	0.17
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	1	0.17
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	19	0.17
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	19	0.17
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	19	0.17
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	19	0.17
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	19	0.17
(1,1552)	1:72:A:GLN:HE22	1:111:A:ARG:HD2	18	0.17
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	19	0.17
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	19	0.17
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	19	0.17
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	8	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	1	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	1	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	1	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	5	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	5	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	5	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	10	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	10	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	10	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	12	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	12	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	12	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	16	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	16	0.17
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	16	0.17
(1,1515)	1:99:A:LYS:HA	1:100:A:ARG:HA	3	0.17
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG2	10	0.17
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG3	10	0.17
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	9	0.17
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	9	0.17
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	9	0.17
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	9	0.17
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	9	0.17
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	9	0.17
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	3	0.17
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	3	0.17
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	3	0.17
(1,1459)	1:48:A:GLU:HB3	1:49:A:ASP:HB3	7	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	1	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	1	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	1	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	5	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	5	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	5	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	10	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	10	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	12	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	12	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	12	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	16	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	16	0.17
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	16	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	5	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	5	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	5	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	10	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	10	0.17
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	10	0.17
(1,1418)	1:7:A:GLN:HG2	1:8:A:PRO:HD3	8	0.17
(1,1418)	1:7:A:GLN:HG3	1:8:A:PRO:HD3	8	0.17
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	13	0.17
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	13	0.17
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	13	0.17
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	2	0.17
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	2	0.17
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	2	0.17
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	20	0.17
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	20	0.17
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	20	0.17
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	14	0.17
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	14	0.17
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	14	0.17
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	20	0.17
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	20	0.17
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	20	0.17
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG2	17	0.17
(1,1072)	1:115:A:GLN:HA	1:115:A:GLN:HG3	17	0.17
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	4	0.17
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	10	0.17
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	18	0.17
(1,981)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	5	0.17
(1,981)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	5	0.17
(1,981)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	5	0.17
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	9	0.17
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	9	0.17
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	9	0.17
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	17	0.17
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	17	0.17
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	19	0.17
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	19	0.17
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	19	0.17
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	19	0.17
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	19	0.17
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	19	0.17
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	6	0.17
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	6	0.17
(1,850)	1:95:A:LYS:HE2	1:99:A:LYS:HB3	3	0.17
(1,850)	1:95:A:LYS:HE3	1:99:A:LYS:HB3	3	0.17
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	15	0.17
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	15	0.17
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	15	0.17
(1,759)	1:67:A:GLU:HG3	1:68:A:ILE:H	13	0.17
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	2	0.17
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	15	0.17
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	3	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	1	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	1	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	1	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	17	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	17	0.17
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	17	0.17
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	19	0.17
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD2	2	0.17
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD3	2	0.17
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	4	0.17
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	4	0.17
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	9	0.17
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	9	0.17
(1,550)	1:51:A:THR:HG21	1:52:A:ASP:H	7	0.17
(1,550)	1:51:A:THR:HG22	1:52:A:ASP:H	7	0.17
(1,550)	1:51:A:THR:HG23	1:52:A:ASP:H	7	0.17
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	1	0.17
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	11	0.17
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	16	0.17
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	18	0.17
(1,462)	1:44:A:ASN:H	1:45:A:PRO:HB2	8	0.17
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	8	0.17
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	4	0.17
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	4	0.17
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	5	0.17
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	5	0.17
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	5	0.17
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	8	0.17
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	8	0.17
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	8	0.17
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	1	0.17
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	1	0.17
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	1	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	13	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	13	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	15	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	15	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	19	0.17
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	19	0.17
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	7	0.17
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	7	0.17
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	7	0.17
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	9	0.17
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	13	0.17
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	13	0.17
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	16	0.17
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	16	0.17
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	7	0.17
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	7	0.17
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	2	0.17
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	2	0.17
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	2	0.17
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	3	0.17
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	3	0.17
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	3	0.17
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	8	0.17
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	8	0.17
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	8	0.17
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	11	0.17
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	11	0.17
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	11	0.17
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	20	0.17
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	20	0.17
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	20	0.17
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	20	0.17
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	20	0.17
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	20	0.17
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	20	0.17
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	20	0.17
(1,55)	1:4:A:ILE:HB	1:5:A:PRO:HD3	15	0.17
(1,14)	1:15:A:ARG:HD2	1:16:A:VAL:HA	5	0.17
(1,14)	1:15:A:ARG:HD3	1:16:A:VAL:HA	5	0.17
(2,61)	1:55:A:ILE:N	1:77:A:ILE:O	1	0.16
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	10	0.16
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	9	0.16
(2,21)	1:34:A:GLY:O	1:56:A:TYR:H	14	0.16
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	19	0.16
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	3	0.16
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	9	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	12	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	12	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	12	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	16	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	16	0.16
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	16	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	11	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	11	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	11	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	17	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	17	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	17	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	20	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	20	0.16
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	20	0.16
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	7	0.16
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	7	0.16
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	7	0.16
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	9	0.16
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	9	0.16
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	9	0.16
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	4	0.16
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	17	0.16
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	17	0.16
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	17	0.16
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	17	0.16
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	17	0.16
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	18	0.16
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	19	0.16
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	19	0.16
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	19	0.16
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	19	0.16
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	19	0.16
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	19	0.16
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	20	0.16
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	19	0.16
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	2	0.16
(1,3131)	1:36:A:GLY:H	1:90:A:HIS:HB2	12	0.16
(1,3128)	1:85:A:MET:HE1	1:92:A:GLN:HE22	3	0.16
(1,3128)	1:85:A:MET:HE2	1:92:A:GLN:HE22	3	0.16
(1,3128)	1:85:A:MET:HE3	1:92:A:GLN:HE22	3	0.16
(1,3120)	1:72:A:GLN:HE21	1:115:A:GLN:HA	19	0.16
(1,3117)	1:48:A:GLU:HB3	1:52:A:ASP:H	10	0.16
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	15	0.16
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	15	0.16
(1,3064)	1:52:A:ASP:HA	1:54:A:GLY:H	19	0.16
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	16	0.16
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	16	0.16
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	16	0.16
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	10	0.16
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	10	0.16
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	5	0.16
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	6	0.16
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	19	0.16
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	3	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	7	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	7	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	7	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	13	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	13	0.16
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	13	0.16
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	19	0.16
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	19	0.16
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	4	0.16
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	9	0.16
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	11	0.16
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	6	0.16
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	9	0.16
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	16	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	7	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	7	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	7	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	9	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	9	0.16
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	9	0.16
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	14	0.16
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	9	0.16
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	10	0.16
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	16	0.16
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	16	0.16
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	16	0.16
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	16	0.16
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD2	2	0.16
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD3	2	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	8	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	8	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	8	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	8	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	8	0.16
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	8	0.16
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	2	0.16
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	2	0.16
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	2	0.16
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	8	0.16
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	15	0.16
(1,2816)	1:23:A:GLN:HB2	1:26:A:ASN:HD21	1	0.16
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	11	0.16
(1,2767)	1:118:A:VAL:HG11	1:119:A:GLN:HE22	11	0.16
(1,2767)	1:118:A:VAL:HG12	1:119:A:GLN:HE22	11	0.16
(1,2767)	1:118:A:VAL:HG13	1:119:A:GLN:HE22	11	0.16
(1,2767)	1:118:A:VAL:HG21	1:119:A:GLN:HE22	11	0.16
(1,2767)	1:118:A:VAL:HG22	1:119:A:GLN:HE22	11	0.16
(1,2767)	1:118:A:VAL:HG23	1:119:A:GLN:HE22	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2736)	1:119:A:GLN:H	1:119:A:GLN:HB3	15	0.16
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	6	0.16
(1,2677)	1:112:A:GLN:H	1:113:A:SER:HB2	18	0.16
(1,2677)	1:112:A:GLN:H	1:113:A:SER:HB3	18	0.16
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	12	0.16
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	14	0.16
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	14	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	1	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	1	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	1	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	8	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	8	0.16
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	8	0.16
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	16	0.16
(1,2564)	1:95:A:LYS:HE2	1:99:A:LYS:H	12	0.16
(1,2564)	1:95:A:LYS:HE3	1:99:A:LYS:H	12	0.16
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	10	0.16
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	10	0.16
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	5	0.16
(1,2450)	1:89:A:THR:H	1:92:A:GLN:HE22	12	0.16
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	5	0.16
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	5	0.16
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	16	0.16
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	17	0.16
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	17	0.16
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	4	0.16
(1,2098)	1:49:A:ASP:HB3	1:50:A:LYS:H	13	0.16
(1,2098)	1:49:A:ASP:HB3	1:50:A:LYS:H	17	0.16
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	6	0.16
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	6	0.16
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	20	0.16
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	1	0.16
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	3	0.16
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	10	0.16
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	13	0.16
(1,1680)	1:112:A:GLN:HB2	1:113:A:SER:H	18	0.16
(1,1677)	1:35:A:GLY:HA3	1:56:A:TYR:H	19	0.16
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	6	0.16
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	11	0.16
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	11	0.16
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	11	0.16
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	14	0.16
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	14	0.16
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	20	0.16
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	20	0.16
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	20	0.16
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	15	0.16
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	15	0.16
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	12	0.16
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	2	0.16
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	2	0.16
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	10	0.16
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	10	0.16
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	10	0.16
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	5	0.16
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	5	0.16
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	5	0.16
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	2	0.16
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	2	0.16
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	2	0.16
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	2	0.16
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	2	0.16
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	2	0.16
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	2	0.16
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	2	0.16
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	2	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	2	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	2	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	10	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	10	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	12	0.16
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	12	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	13	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	13	0.16
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	13	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	13	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	13	0.16
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	13	0.16
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	9	0.16
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	9	0.16
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	9	0.16
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	7	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	3	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	3	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	13	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	13	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	13	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	19	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	19	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	19	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	20	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	20	0.16
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	20	0.16
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD11	16	0.16
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD12	16	0.16
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD13	16	0.16
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD11	16	0.16
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD12	16	0.16
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD13	16	0.16
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD11	16	0.16
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD12	16	0.16
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD13	16	0.16
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	16	0.16
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	16	0.16
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	16	0.16
(1,1458)	1:23:A:GLN:HB2	1:26:A:ASN:HB2	6	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD11	8	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD12	8	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD13	8	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD21	8	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD22	8	0.16
(1,1448)	1:20:A:LYS:HA	1:27:A:LEU:HD23	8	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	3	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	3	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	3	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	13	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	13	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	13	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	15	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	15	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	15	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	19	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	19	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	20	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	20	0.16
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	20	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	13	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	13	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	13	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	17	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	17	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	17	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	18	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	18	0.16
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	18	0.16
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	14	0.16
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	14	0.16
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	14	0.16
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	9	0.16
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	9	0.16
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	9	0.16
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	10	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	7	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	7	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	7	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	11	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	11	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	11	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	15	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	15	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	15	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	16	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	16	0.16
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	16	0.16
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	6	0.16
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	6	0.16
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	6	0.16
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	6	0.16
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	6	0.16
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	6	0.16
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	8	0.16
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	8	0.16
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	8	0.16
(1,1217)	1:86:A:THR:H	1:86:A:THR:HG21	5	0.16
(1,1217)	1:86:A:THR:H	1:86:A:THR:HG22	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1217)	1:86:A:THR:H	1:86:A:THR:HG23	5	0.16
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	11	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	2	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	3	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	5	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	6	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	8	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	13	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	17	0.16
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	19	0.16
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	7	0.16
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	7	0.16
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	7	0.16
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	1	0.16
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	1	0.16
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	1	0.16
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	7	0.16
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	7	0.16
(1,850)	1:95:A:LYS:HE2	1:99:A:LYS:HB3	14	0.16
(1,850)	1:95:A:LYS:HE3	1:99:A:LYS:HB3	14	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	11	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	11	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	11	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	16	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	16	0.16
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	16	0.16
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	13	0.16
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	8	0.16
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	8	0.16
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	8	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	4	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	4	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	4	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	13	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	13	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	13	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	15	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	15	0.16
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	15	0.16
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	20	0.16
(1,513)	1:46:A:PHE:H	1:47:A:SER:HB3	2	0.16
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG2	2	0.16
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG3	2	0.16
(1,437)	1:4:A:ILE:HA	1:5:A:PRO:HG3	12	0.16
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	6	0.16
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	14	0.16
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	16	0.16
(1,359)	1:36:A:GLY:HA3	1:37:A:ILE:HG13	14	0.16
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	19	0.16
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	19	0.16
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	19	0.16
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	6	0.16
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	6	0.16
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	6	0.16
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	16	0.16
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	18	0.16
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	17	0.16
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	3	0.16
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	3	0.16
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	7	0.16
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG21	1	0.16
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG22	1	0.16
(1,12)	1:50:A:LYS:HD2	1:51:A:THR:HG23	1	0.16
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG21	1	0.16
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG22	1	0.16
(1,12)	1:50:A:LYS:HD3	1:51:A:THR:HG23	1	0.16
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	19	0.15
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	4	0.15
(2,56)	1:55:A:ILE:O	1:77:A:ILE:H	6	0.15
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	14	0.15
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	1	0.15
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	2	0.15
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	1	0.15
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	1	0.15
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	1	0.15
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	7	0.15
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	7	0.15
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	7	0.15
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	6	0.15
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	5	0.15
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	4	0.15
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	4	0.15
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	4	0.15
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	4	0.15
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	4	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	13	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	13	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	13	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	13	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	13	0.15
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	13	0.15
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	13	0.15
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	13	0.15
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	16	0.15
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	2	0.15
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	15	0.15
(1,3138)	1:14:A:GLN:H	1:111:A:ARG:HD2	20	0.15
(1,3134)	1:78:A:MET:HA	1:110:A:THR:H	5	0.15
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	4	0.15
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	13	0.15
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	13	0.15
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	13	0.15
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	15	0.15
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	15	0.15
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	15	0.15
(1,3120)	1:72:A:GLN:HE21	1:115:A:GLN:HA	12	0.15
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD2	18	0.15
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD3	18	0.15
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	5	0.15
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	5	0.15
(1,3103)	1:89:A:THR:H	1:92:A:GLN:HA	8	0.15
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	9	0.15
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	9	0.15
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	18	0.15
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	18	0.15
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	18	0.15
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	17	0.15
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	17	0.15
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	17	0.15
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	18	0.15
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	18	0.15
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	18	0.15
(1,3062)	1:52:A:ASP:HB2	1:54:A:GLY:H	5	0.15
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	20	0.15
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	20	0.15
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	1	0.15
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	10	0.15
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	13	0.15
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	14	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	4	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	4	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	4	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	18	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	18	0.15
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	18	0.15
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	1	0.15
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	20	0.15
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	20	0.15
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	20	0.15
(1,2994)	1:18:A:ILE:H	1:20:A:LYS:H	16	0.15
(1,2987)	1:4:A:ILE:H	1:8:A:PRO:HD3	1	0.15
(1,2985)	1:14:A:GLN:H	1:14:A:GLN:HE22	9	0.15
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	1	0.15
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	4	0.15
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	1	0.15
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	1	0.15
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	18	0.15
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	4	0.15
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	6	0.15
(1,2958)	1:72:A:GLN:HE22	1:111:A:ARG:H	4	0.15
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	13	0.15
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	13	0.15
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	13	0.15
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	13	0.15
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	13	0.15
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	15	0.15
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	15	0.15
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	15	0.15
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	15	0.15
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	15	0.15
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	5	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	7	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	15	0.15
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	15	0.15
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	6	0.15
(1,2852)	1:56:A:TYR:HD1	1:75:A:ASP:H	14	0.15
(1,2852)	1:56:A:TYR:HD2	1:75:A:ASP:H	14	0.15
(1,2848)	1:57:A:VAL:HG21	1:74:A:GLY:H	20	0.15
(1,2848)	1:57:A:VAL:HG22	1:74:A:GLY:H	20	0.15
(1,2848)	1:57:A:VAL:HG23	1:74:A:GLY:H	20	0.15
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	2	0.15
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	3	0.15
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	4	0.15
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	11	0.15
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	6	0.15
(1,2787)	1:19:A:HIS:H	1:65:A:PRO:HB3	15	0.15
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	5	0.15
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	1	0.15
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	1	0.15
(1,2762)	1:82:A:GLY:H	1:106:A:ARG:H	18	0.15
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:116:A:LYS:HA	1:117:A:ALA:H	2	0.15
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	9	0.15
(1,2682)	1:110:A:THR:HG21	1:112:A:GLN:HE21	8	0.15
(1,2682)	1:110:A:THR:HG22	1:112:A:GLN:HE21	8	0.15
(1,2682)	1:110:A:THR:HG23	1:112:A:GLN:HE21	8	0.15
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	13	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	3	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	3	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	3	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	16	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	16	0.15
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	16	0.15
(1,2566)	1:97:A:LEU:HD11	1:99:A:LYS:H	7	0.15
(1,2566)	1:97:A:LEU:HD12	1:99:A:LYS:H	7	0.15
(1,2566)	1:97:A:LEU:HD13	1:99:A:LYS:H	7	0.15
(1,2566)	1:97:A:LEU:HD21	1:99:A:LYS:H	7	0.15
(1,2566)	1:97:A:LEU:HD22	1:99:A:LYS:H	7	0.15
(1,2566)	1:97:A:LEU:HD23	1:99:A:LYS:H	7	0.15
(1,2452)	1:36:A:GLY:HA2	1:90:A:HIS:H	19	0.15
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	20	0.15
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	6	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	5	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	5	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	5	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	13	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	13	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	13	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	19	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	19	0.15
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	19	0.15
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	2	0.15
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	2	0.15
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	4	0.15
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	4	0.15
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	11	0.15
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	11	0.15
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	5	0.15
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	9	0.15
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	13	0.15
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD2	3	0.15
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD3	3	0.15
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	16	0.15
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	20	0.15
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	20	0.15
(1,2052)	1:44:A:ASN:H	1:45:A:PRO:HD2	6	0.15
(1,2038)	1:43:A:GLN:HA	1:43:A:GLN:HE22	15	0.15
(1,1884)	1:29:A:LEU:HG	1:31:A:PHE:H	5	0.15
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	3	0.15
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	12	0.15
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	2	0.15
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	18	0.15
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	1	0.15
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	10	0.15
(1,1667)	1:14:A:GLN:HA	1:14:A:GLN:HE22	9	0.15
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	20	0.15
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	20	0.15
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	8	0.15
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	8	0.15
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	8	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	4	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	5	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	8	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	9	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	10	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	11	0.15
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	19	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	3	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	3	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	3	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	5	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	5	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	5	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	19	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	19	0.15
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	19	0.15
(1,1633)	1:14:A:GLN:H	1:111:A:ARG:HD3	17	0.15
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	11	0.15
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	11	0.15
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	11	0.15
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	4	0.15
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	4	0.15
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	5	0.15
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	9	0.15
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	9	0.15
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	14	0.15
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	14	0.15
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	18	0.15
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	18	0.15
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	17	0.15
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	17	0.15
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	17	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	13	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	13	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	13	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	18	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	18	0.15
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	18	0.15
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	1	0.15
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	14	0.15
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	13	0.15
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	13	0.15
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	13	0.15
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	10	0.15
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	10	0.15
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	10	0.15
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	10	0.15
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	10	0.15
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	10	0.15
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	5	0.15
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	5	0.15
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	5	0.15
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	9	0.15
(1,1536)	1:13:A:VAL:HA	1:110:A:THR:HA	5	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	9	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	9	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	9	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	14	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	14	0.15
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	14	0.15
(1,1521)	1:19:A:HIS:HB3	1:104:A:VAL:HG21	9	0.15
(1,1521)	1:19:A:HIS:HB3	1:104:A:VAL:HG22	9	0.15
(1,1521)	1:19:A:HIS:HB3	1:104:A:VAL:HG23	9	0.15
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG2	16	0.15
(1,1503)	1:71:A:LEU:HG	1:72:A:GLN:HG3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	14	0.15
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	14	0.15
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	14	0.15
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	15	0.15
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	15	0.15
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	15	0.15
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	2	0.15
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	2	0.15
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	2	0.15
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	2	0.15
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	2	0.15
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	2	0.15
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	8	0.15
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	8	0.15
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	8	0.15
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	12	0.15
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	12	0.15
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	12	0.15
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	18	0.15
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	18	0.15
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	18	0.15
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	6	0.15
(1,1435)	1:16:A:VAL:HB	1:107:A:LEU:HG	17	0.15
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	9	0.15
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	9	0.15
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	9	0.15
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	8	0.15
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	8	0.15
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	8	0.15
(1,1418)	1:7:A:GLN:HG2	1:8:A:PRO:HD3	16	0.15
(1,1418)	1:7:A:GLN:HG3	1:8:A:PRO:HD3	16	0.15
(1,1408)	1:34:A:GLY:HA3	1:90:A:HIS:HE1	12	0.15
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	3	0.15
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	3	0.15
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	3	0.15
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	7	0.15
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	7	0.15
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	7	0.15
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	13	0.15
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	13	0.15
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	13	0.15
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	15	0.15
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	15	0.15
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	8	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	9	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	9	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	9	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	10	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	10	0.15
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	10	0.15
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	15	0.15
(1,1019)	1:50:A:LYS:HB2	1:110:A:THR:HG21	2	0.15
(1,1019)	1:50:A:LYS:HB2	1:110:A:THR:HG22	2	0.15
(1,1019)	1:50:A:LYS:HB2	1:110:A:THR:HG23	2	0.15
(1,1019)	1:50:A:LYS:HB3	1:110:A:THR:HG21	2	0.15
(1,1019)	1:50:A:LYS:HB3	1:110:A:THR:HG22	2	0.15
(1,1019)	1:50:A:LYS:HB3	1:110:A:THR:HG23	2	0.15
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	1	0.15
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	1	0.15
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	1	0.15
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	20	0.15
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	20	0.15
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	20	0.15
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	8	0.15
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	8	0.15
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	8	0.15
(1,760)	1:60:A:VAL:HG11	1:67:A:GLU:HG2	7	0.15
(1,760)	1:60:A:VAL:HG12	1:67:A:GLU:HG2	7	0.15
(1,760)	1:60:A:VAL:HG13	1:67:A:GLU:HG2	7	0.15
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	9	0.15
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	9	0.15
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	9	0.15
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	18	0.15
(1,661)	1:60:A:VAL:HG11	1:61:A:SER:HB3	19	0.15
(1,661)	1:60:A:VAL:HG12	1:61:A:SER:HB3	19	0.15
(1,661)	1:60:A:VAL:HG13	1:61:A:SER:HB3	19	0.15
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	1	0.15
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	16	0.15
(1,523)	1:47:A:SER:HB3	1:49:A:ASP:H	17	0.15
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	2	0.15
(1,475)	1:44:A:ASN:H	1:45:A:PRO:HD2	6	0.15
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	3	0.15
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	15	0.15
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	15	0.15
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	15	0.15
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	7	0.15
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	6	0.15
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	6	0.15
(1,223)	1:18:A:ILE:HG21	1:19:A:HIS:HB3	13	0.15
(1,223)	1:18:A:ILE:HG22	1:19:A:HIS:HB3	13	0.15
(1,223)	1:18:A:ILE:HG23	1:19:A:HIS:HB3	13	0.15
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	3	0.15
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	3	0.15
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	13	0.15
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	13	0.15
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	13	0.15
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	13	0.15
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	13	0.15
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	13	0.15
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	6	0.14
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	2	0.14
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	3	0.14
(2,22)	1:36:A:GLY:H	1:54:A:GLY:O	3	0.14
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	12	0.14
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	20	0.14
(1,3189)	1:44:A:ASN:H	1:47:A:SER:H	15	0.14
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	4	0.14
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	4	0.14
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	4	0.14
(1,3186)	1:14:A:GLN:HG2	1:109:A:VAL:HB	6	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	1	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	1	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	1	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	3	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	3	0.14
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	3	0.14
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	17	0.14
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	17	0.14
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	17	0.14
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	9	0.14
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	15	0.14
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	1	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	17	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	17	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	17	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	17	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	17	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	17	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	17	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	17	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	19	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	19	0.14
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	19	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	19	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	19	0.14
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	19	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	19	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	19	0.14
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	19	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	3	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	3	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	3	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	3	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	3	0.14
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	3	0.14
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	3	0.14
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	3	0.14
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	16	0.14
(1,3138)	1:14:A:GLN:H	1:111:A:ARG:HD2	1	0.14
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	14	0.14
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	14	0.14
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	14	0.14
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	7	0.14
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	7	0.14
(1,3103)	1:89:A:THR:H	1:92:A:GLN:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	13	0.14
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	13	0.14
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	13	0.14
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	16	0.14
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	16	0.14
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	16	0.14
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	20	0.14
(1,3093)	1:24:A:GLY:HA2	1:25:A:GLU:HG3	12	0.14
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	10	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	2	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	2	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	2	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	3	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	3	0.14
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	3	0.14
(1,3064)	1:52:A:ASP:HA	1:54:A:GLY:H	15	0.14
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	2	0.14
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	9	0.14
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	16	0.14
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	17	0.14
(1,3037)	1:35:A:GLY:H	1:39:A:GLN:HG3	12	0.14
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	11	0.14
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	15	0.14
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	1	0.14
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	2	0.14
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	9	0.14
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	20	0.14
(1,3022)	1:47:A:SER:H	1:48:A:GLU:HB2	19	0.14
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	12	0.14
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	12	0.14
(1,2983)	1:37:A:ILE:H	1:87:A:MET:HB2	12	0.14
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	17	0.14
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	5	0.14
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	11	0.14
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	11	0.14
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	16	0.14
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	14	0.14
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	1	0.14
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	10	0.14
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	14	0.14
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	14	0.14
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	14	0.14
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	14	0.14
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	14	0.14
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	14	0.14
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	14	0.14
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	14	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	12	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	12	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	12	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	12	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	12	0.14
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	12	0.14
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	5	0.14
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	5	0.14
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	5	0.14
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD11	2	0.14
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD12	2	0.14
(1,2844)	1:72:A:GLN:HE22	1:114:A:LEU:HD13	2	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD11	11	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD12	11	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD13	11	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD21	11	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD22	11	0.14
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD23	11	0.14
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	5	0.14
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	13	0.14
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	11	0.14
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	17	0.14
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	19	0.14
(1,2765)	1:72:A:GLN:HE22	1:112:A:GLN:H	12	0.14
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	3	0.14
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	3	0.14
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	13	0.14
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	13	0.14
(1,2736)	1:119:A:GLN:H	1:119:A:GLN:HB3	6	0.14
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	16	0.14
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	12	0.14
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	12	0.14
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	12	0.14
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	7	0.14
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	7	0.14
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	20	0.14
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	20	0.14
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	20	0.14
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD21	13	0.14
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD22	13	0.14
(1,2702)	1:114:A:LEU:H	1:114:A:LEU:HD23	13	0.14
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	5	0.14
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	6	0.14
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	16	0.14
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	16	0.14
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	10	0.14
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	10	0.14
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	10	0.14
(1,2578)	1:99:A:LYS:HG2	1:100:A:ARG:H	1	0.14
(1,2564)	1:95:A:LYS:HE2	1:99:A:LYS:H	11	0.14
(1,2564)	1:95:A:LYS:HE3	1:99:A:LYS:H	11	0.14
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	12	0.14
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	12	0.14
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	19	0.14
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	7	0.14
(1,2370)	1:79:A:GLN:HA	1:79:A:GLN:HE22	15	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	2	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	2	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	2	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	10	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	10	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	10	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	14	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	14	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	14	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	20	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	20	0.14
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	20	0.14
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	11	0.14
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	11	0.14
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	19	0.14
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	19	0.14
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	10	0.14
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	10	0.14
(1,2311)	1:72:A:GLN:H	1:72:A:GLN:HE22	10	0.14
(1,2255)	1:67:A:GLU:H	1:68:A:ILE:HG13	14	0.14
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	9	0.14
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	20	0.14
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD2	1	0.14
(1,2091)	1:49:A:ASP:H	1:50:A:LYS:HD3	1	0.14
(1,2067)	1:44:A:ASN:HB2	1:47:A:SER:H	18	0.14
(1,2043)	1:41:A:PRO:HA	1:44:A:ASN:H	6	0.14
(1,1992)	1:39:A:GLN:HA	1:39:A:GLN:HE22	5	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	4	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	19	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	19	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	19	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	19	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	19	0.14
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	19	0.14
(1,1757)	1:15:A:ARG:H	1:15:A:ARG:HB3	18	0.14
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG21	12	0.14
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG22	12	0.14
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG23	12	0.14
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	9	0.14
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	9	0.14
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	19	0.14
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	19	0.14
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	15	0.14
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	15	0.14
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	15	0.14
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	7	0.14
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	17	0.14
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	20	0.14
(1,1633)	1:14:A:GLN:H	1:111:A:ARG:HD3	13	0.14
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	9	0.14
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	9	0.14
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	15	0.14
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	15	0.14
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	7	0.14
(1,1578)	1:79:A:GLN:HB2	1:108:A:LEU:HB2	13	0.14
(1,1578)	1:79:A:GLN:HB2	1:108:A:LEU:HB3	13	0.14
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG21	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG22	12	0.14
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG23	12	0.14
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG21	12	0.14
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG22	12	0.14
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG23	12	0.14
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG21	12	0.14
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG22	12	0.14
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG23	12	0.14
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	7	0.14
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	7	0.14
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	7	0.14
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	7	0.14
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	7	0.14
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	7	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	11	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	11	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	11	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	11	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	11	0.14
(1,1560)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	11	0.14
(1,1560)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	11	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	8	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	8	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	8	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	11	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	11	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	11	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	20	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	20	0.14
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	20	0.14
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	7	0.14
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	7	0.14
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	7	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	7	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	7	0.14
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	7	0.14
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	7	0.14
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	7	0.14
(1,1523)	1:18:A:ILE:H	1:105:A:VAL:HG11	14	0.14
(1,1523)	1:18:A:ILE:H	1:105:A:VAL:HG12	14	0.14
(1,1523)	1:18:A:ILE:H	1:105:A:VAL:HG13	14	0.14
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	7	0.14
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD11	12	0.14
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD12	12	0.14
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD13	12	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD11	12	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD12	12	0.14
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD13	12	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD11	12	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD12	12	0.14
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD13	12	0.14
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	6	0.14
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	6	0.14
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	6	0.14
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	6	0.14
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	6	0.14
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	6	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD11	11	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD12	11	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD13	11	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD21	11	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD22	11	0.14
(1,1433)	1:15:A:ARG:HD2	1:108:A:LEU:HD23	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD11	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD12	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD13	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD21	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD22	11	0.14
(1,1433)	1:15:A:ARG:HD3	1:108:A:LEU:HD23	11	0.14
(1,1408)	1:34:A:GLY:HA3	1:90:A:HIS:HE1	5	0.14
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	1	0.14
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	1	0.14
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	1	0.14
(1,1309)	1:88:A:VAL:HA	1:92:A:GLN:HB2	5	0.14
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	13	0.14
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	13	0.14
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	13	0.14
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	8	0.14
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	8	0.14
(1,1220)	1:86:A:THR:HG21	1:87:A:MET:HG3	14	0.14
(1,1220)	1:86:A:THR:HG22	1:87:A:MET:HG3	14	0.14
(1,1220)	1:86:A:THR:HG23	1:87:A:MET:HG3	14	0.14
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	1	0.14
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	1	0.14
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	1	0.14
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	7	0.14
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	7	0.14
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	7	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD21	5	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD22	5	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD23	5	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD21	20	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD22	20	0.14
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD23	20	0.14
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	1	0.14
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	12	0.14
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	12	0.14
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	12	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	3	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	3	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	3	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	7	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	7	0.14
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	7	0.14
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	6	0.14
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	6	0.14
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	6	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	16	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	16	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	16	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	18	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	18	0.14
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	18	0.14
(1,751)	1:67:A:GLU:HA	1:67:A:GLU:HG2	11	0.14
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	7	0.14
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	7	0.14
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	7	0.14
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	9	0.14
(1,681)	1:62:A:GLU:HG2	1:63:A:GLY:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	2	0.14
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	4	0.14
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	17	0.14
(1,608)	1:32:A:SER:HB2	1:59:A:ARG:HB2	2	0.14
(1,512)	1:47:A:SER:HB3	1:52:A:ASP:HB2	11	0.14
(1,510)	1:44:A:ASN:HB2	1:47:A:SER:HB3	17	0.14
(1,503)	1:46:A:PHE:H	1:47:A:SER:HA	16	0.14
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG2	15	0.14
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG3	15	0.14
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	7	0.14
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	7	0.14
(1,402)	1:39:A:GLN:HA	1:39:A:GLN:HG3	10	0.14
(1,316)	1:32:A:SER:HB2	1:33:A:ILE:H	14	0.14
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	20	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	4	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	9	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	10	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	11	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	18	0.14
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	20	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	11	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	11	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	17	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	17	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	20	0.14
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	20	0.14
(1,235)	1:21:A:LEU:HA	1:22:A:ARG:HB3	8	0.14
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	11	0.14
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	11	0.14
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	11	0.14
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	11	0.14
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	11	0.14
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	11	0.14
(1,87)	1:8:A:PRO:HA	1:9:A:VAL:H	10	0.14
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	17	0.14
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	2	0.13
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	8	0.13
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	17	0.13
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	19	0.13
(2,37)	1:21:A:LEU:N	1:28:A:ILE:O	11	0.13
(2,15)	1:92:A:GLN:O	1:96:A:ARG:H	1	0.13
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	10	0.13
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	18	0.13
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	9	0.13
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	9	0.13
(1,3184)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	9	0.13
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	3	0.13
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	3	0.13
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	3	0.13
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	12	0.13
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	5	0.13
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	6	0.13
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	12	0.13
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	15	0.13
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	5	0.13
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	5	0.13
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	5	0.13
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	5	0.13
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	5	0.13
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	5	0.13
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	5	0.13
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	5	0.13
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	5	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	20	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	20	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	20	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	20	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	20	0.13
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	20	0.13
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	20	0.13
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	20	0.13
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	7	0.13
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3144)	1:57:A:VAL:H	1:77:A:ILE:HA	14	0.13
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	1	0.13
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	13	0.13
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	9	0.13
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	16	0.13
(1,3113)	1:38:A:ASP:HA	1:89:A:THR:H	8	0.13
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	1	0.13
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	1	0.13
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	1	0.13
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	4	0.13
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	4	0.13
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	4	0.13
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	15	0.13
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	15	0.13
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	15	0.13
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	20	0.13
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	20	0.13
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	20	0.13
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	14	0.13
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	6	0.13
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	6	0.13
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	6	0.13
(1,3071)	1:68:A:ILE:HD11	1:70:A:GLY:H	16	0.13
(1,3071)	1:68:A:ILE:HD12	1:70:A:GLY:H	16	0.13
(1,3071)	1:68:A:ILE:HD13	1:70:A:GLY:H	16	0.13
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	11	0.13
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	18	0.13
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	18	0.13
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	18	0.13
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	19	0.13
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	19	0.13
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	19	0.13
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	20	0.13
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	20	0.13
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	20	0.13
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	11	0.13
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	13	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	8	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	8	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	9	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	9	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	13	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB2	16	0.13
(1,3035)	1:35:A:GLY:H	1:39:A:GLN:HB3	16	0.13
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	4	0.13
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	7	0.13
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	9	0.13
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	15	0.13
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	4	0.13
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	15	0.13
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	17	0.13
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB1	9	0.13
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB2	9	0.13
(1,3029)	1:16:A:VAL:H	1:69:A:ALA:HB3	9	0.13
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	13	0.13
(1,3019)	1:19:A:HIS:HB2	1:105:A:VAL:H	13	0.13
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	2	0.13
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	2	0.13
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	12	0.13
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	12	0.13
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	14	0.13
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	14	0.13
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	16	0.13
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	16	0.13
(1,3015)	1:89:A:THR:HG21	1:92:A:GLN:HE22	14	0.13
(1,3015)	1:89:A:THR:HG22	1:92:A:GLN:HE22	14	0.13
(1,3015)	1:89:A:THR:HG23	1:92:A:GLN:HE22	14	0.13
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG12	3	0.13
(1,3007)	1:76:A:LYS:H	1:77:A:ILE:HG13	3	0.13
(1,2986)	1:72:A:GLN:HE22	1:113:A:SER:H	20	0.13
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	10	0.13
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	11	0.13
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	3	0.13
(1,2975)	1:98:A:THR:H	1:99:A:LYS:HB2	4	0.13
(1,2974)	1:97:A:LEU:H	1:97:A:LEU:HG	13	0.13
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	15	0.13
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	15	0.13
(1,2965)	1:22:A:ARG:HG2	1:24:A:GLY:H	12	0.13
(1,2965)	1:22:A:ARG:HG3	1:24:A:GLY:H	12	0.13
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	20	0.13
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	20	0.13
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG11	9	0.13
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG13	9	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	7	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	7	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	7	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	10	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	10	0.13
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	10	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE1	8	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE2	8	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE3	8	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE1	9	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE2	9	0.13
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE3	9	0.13
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD2	15	0.13
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD3	15	0.13
(1,2903)	1:79:A:GLN:HB2	1:83:A:TRP:H	20	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	11	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	11	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	11	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	11	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	11	0.13
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	11	0.13
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	14	0.13
(1,2816)	1:23:A:GLN:HB2	1:26:A:ASN:HD21	6	0.13
(1,2800)	1:20:A:LYS:HE2	1:22:A:ARG:H	2	0.13
(1,2800)	1:20:A:LYS:HE3	1:22:A:ARG:H	2	0.13
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	4	0.13
(1,2773)	1:14:A:GLN:H	1:110:A:THR:HB	15	0.13
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	2	0.13
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	2	0.13
(1,2762)	1:82:A:GLY:H	1:106:A:ARG:H	6	0.13
(1,2762)	1:82:A:GLY:H	1:106:A:ARG:H	14	0.13
(1,2711)	1:114:A:LEU:HD11	1:115:A:GLN:HE21	17	0.13
(1,2711)	1:114:A:LEU:HD12	1:115:A:GLN:HE21	17	0.13
(1,2711)	1:114:A:LEU:HD13	1:115:A:GLN:HE21	17	0.13
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	4	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	2	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	2	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	2	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	12	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	12	0.13
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	1	0.13
(1,2570)	1:99:A:LYS:H	1:99:A:LYS:HB2	17	0.13
(1,2566)	1:97:A:LEU:HD11	1:99:A:LYS:H	2	0.13
(1,2566)	1:97:A:LEU:HD12	1:99:A:LYS:H	2	0.13
(1,2566)	1:97:A:LEU:HD13	1:99:A:LYS:H	2	0.13
(1,2566)	1:97:A:LEU:HD21	1:99:A:LYS:H	2	0.13
(1,2566)	1:97:A:LEU:HD22	1:99:A:LYS:H	2	0.13
(1,2566)	1:97:A:LEU:HD23	1:99:A:LYS:H	2	0.13
(1,2559)	1:97:A:LEU:HG	1:98:A:THR:H	19	0.13
(1,2538)	1:95:A:LYS:H	1:95:A:LYS:HB2	18	0.13
(1,2518)	1:88:A:VAL:HG11	1:94:A:ARG:H	15	0.13
(1,2518)	1:88:A:VAL:HG12	1:94:A:ARG:H	15	0.13
(1,2518)	1:88:A:VAL:HG13	1:94:A:ARG:H	15	0.13
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	7	0.13
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	9	0.13
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	14	0.13
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	15	0.13
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	1	0.13
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	10	0.13
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	9	0.13
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	11	0.13
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	17	0.13
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	15	0.13
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	15	0.13
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	15	0.13
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	16	0.13
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	16	0.13
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	2	0.13
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	15	0.13
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	13	0.13
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	13	0.13
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	2	0.13
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	4	0.13
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	15	0.13
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD2	20	0.13
(1,2127)	1:53:A:LYS:H	1:53:A:LYS:HD3	20	0.13
(1,2029)	1:43:A:GLN:H	1:44:A:ASN:HB3	18	0.13
(1,1884)	1:29:A:LEU:HG	1:31:A:PHE:H	14	0.13
(1,1875)	1:29:A:LEU:H	1:30:A:GLY:HA3	10	0.13
(1,1810)	1:22:A:ARG:H	1:23:A:GLN:HE21	20	0.13
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD11	13	0.13
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD12	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD13	13	0.13
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	10	0.13
(1,1674)	1:39:A:GLN:HB2	1:90:A:HIS:H	5	0.13
(1,1674)	1:39:A:GLN:HB3	1:90:A:HIS:H	5	0.13
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	9	0.13
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	13	0.13
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	17	0.13
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	2	0.13
(1,1664)	1:43:A:GLN:H	1:44:A:ASN:HB2	13	0.13
(1,1662)	1:113:A:SER:HB2	1:114:A:LEU:H	8	0.13
(1,1662)	1:113:A:SER:HB3	1:114:A:LEU:H	8	0.13
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	18	0.13
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	18	0.13
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	1	0.13
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE2	1	0.13
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE3	1	0.13
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	15	0.13
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	15	0.13
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	15	0.13
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	8	0.13
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	8	0.13
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	20	0.13
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	20	0.13
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	12	0.13
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	12	0.13
(1,1623)	1:37:A:ILE:HB	1:87:A:MET:HB3	5	0.13
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	2	0.13
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	2	0.13
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	6	0.13
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	6	0.13
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	2	0.13
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	2	0.13
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	2	0.13
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	5	0.13
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	6	0.13
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	13	0.13
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	19	0.13
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB2	5	0.13
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB3	5	0.13
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	13	0.13
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	13	0.13
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	13	0.13
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	13	0.13
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	13	0.13
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	13	0.13
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	13	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	6	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	6	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	6	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	18	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	18	0.13
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	18	0.13
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	9	0.13
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	9	0.13
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	9	0.13
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	9	0.13
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	9	0.13
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	9	0.13
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	9	0.13
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	9	0.13
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	9	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	4	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	4	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	4	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	7	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	7	0.13
(1,1531)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	7	0.13
(1,1476)	1:58:A:THR:HG21	1:59:A:ARG:HG2	19	0.13
(1,1476)	1:58:A:THR:HG22	1:59:A:ARG:HG2	19	0.13
(1,1476)	1:58:A:THR:HG23	1:59:A:ARG:HG2	19	0.13
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	2	0.13
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	2	0.13
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	2	0.13
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	1	0.13
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	1	0.13
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	1	0.13
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	1	0.13
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	1	0.13
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	1	0.13
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	9	0.13
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	9	0.13
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	9	0.13
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	10	0.13
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	10	0.13
(1,1459)	1:48:A:GLU:HB3	1:49:A:ASP:HB3	13	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	4	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	4	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	4	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG11	7	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG12	7	0.13
(1,1431)	1:14:A:GLN:HG3	1:109:A:VAL:HG13	7	0.13
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	2	0.13
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	2	0.13
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	2	0.13
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	16	0.13
(1,1404)	1:33:A:ILE:HD11	1:90:A:HIS:HE1	1	0.13
(1,1404)	1:33:A:ILE:HD12	1:90:A:HIS:HE1	1	0.13
(1,1404)	1:33:A:ILE:HD13	1:90:A:HIS:HE1	1	0.13
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	16	0.13
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	16	0.13
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	16	0.13
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	18	0.13
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	18	0.13
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	18	0.13
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	6	0.13
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	6	0.13
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	6	0.13
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	14	0.13
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	14	0.13
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	14	0.13
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG21	12	0.13
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG22	12	0.13
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG23	12	0.13
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	13	0.13
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	14	0.13
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	4	0.13
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	4	0.13
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	4	0.13
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	13	0.13
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	11	0.13
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	11	0.13
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	11	0.13
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	12	0.13
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	12	0.13
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	15	0.13
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	15	0.13
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	15	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	2	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	2	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	2	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	4	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	4	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	4	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	8	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	8	0.13
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	8	0.13
(1,957)	1:103:A:GLU:HB2	1:104:A:VAL:HG11	9	0.13
(1,957)	1:103:A:GLU:HB2	1:104:A:VAL:HG12	9	0.13
(1,957)	1:103:A:GLU:HB2	1:104:A:VAL:HG13	9	0.13
(1,957)	1:103:A:GLU:HB3	1:104:A:VAL:HG11	9	0.13
(1,957)	1:103:A:GLU:HB3	1:104:A:VAL:HG12	9	0.13
(1,957)	1:103:A:GLU:HB3	1:104:A:VAL:HG13	9	0.13
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	10	0.13
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	10	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	1	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	1	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	1	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	4	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	4	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	4	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	9	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	9	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	9	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	17	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	17	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	17	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	18	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	18	0.13
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	18	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	8	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	8	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	8	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	17	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	17	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	20	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	20	0.13
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	20	0.13
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	20	0.13
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	20	0.13
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	20	0.13
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	11	0.13
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	12	0.13
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD2	20	0.13
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD3	20	0.13
(1,551)	1:52:A:ASP:HA	1:53:A:LYS:H	10	0.13
(1,534)	1:48:A:GLU:H	1:48:A:GLU:HG3	13	0.13
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	14	0.13
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG2	20	0.13
(1,446)	1:43:A:GLN:HA	1:43:A:GLN:HG3	20	0.13
(1,424)	1:40:A:ASP:HB2	1:41:A:PRO:HD2	1	0.13
(1,411)	1:39:A:GLN:HG2	1:90:A:HIS:HB3	5	0.13
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	3	0.13
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	3	0.13
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	3	0.13
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	13	0.13
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	13	0.13
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	13	0.13
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	11	0.13
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	11	0.13
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	11	0.13
(1,320)	1:32:A:SER:HB2	1:59:A:ARG:HA	17	0.13
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	9	0.13
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	9	0.13
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	9	0.13
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	6	0.13
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	8	0.13
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	13	0.13
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	16	0.13
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	5	0.13
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	5	0.13
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	8	0.13
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	8	0.13
(1,235)	1:21:A:LEU:HA	1:22:A:ARG:HB3	6	0.13
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	9	0.13
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	9	0.13
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	10	0.13
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	10	0.13
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	10	0.13
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	10	0.13
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	10	0.13
(2,57)	1:59:A:ARG:H	1:73:A:ILE:O	11	0.12
(2,15)	1:92:A:GLN:O	1:96:A:ARG:H	9	0.12
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG21	17	0.12
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG22	17	0.12
(1,3188)	1:18:A:ILE:H	1:105:A:VAL:HG23	17	0.12
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG11	5	0.12
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG12	5	0.12
(1,3187)	1:15:A:ARG:HA	1:109:A:VAL:HG13	5	0.12
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	8	0.12
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	8	0.12
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	8	0.12
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	2	0.12
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	3	0.12
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	11	0.12
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	2	0.12
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	4	0.12
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	9	0.12
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	11	0.12
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	3	0.12
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	3	0.12
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	3	0.12
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	3	0.12
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	3	0.12
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	3	0.12
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	3	0.12
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	3	0.12
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	3	0.12
(1,3152)	1:27:A:LEU:HB2	1:98:A:THR:HG21	7	0.12
(1,3152)	1:27:A:LEU:HB2	1:98:A:THR:HG22	7	0.12
(1,3152)	1:27:A:LEU:HB2	1:98:A:THR:HG23	7	0.12
(1,3152)	1:27:A:LEU:HB3	1:98:A:THR:HG21	7	0.12
(1,3152)	1:27:A:LEU:HB3	1:98:A:THR:HG22	7	0.12
(1,3152)	1:27:A:LEU:HB3	1:98:A:THR:HG23	7	0.12
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	2	0.12
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	2	0.12
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	2	0.12
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	2	0.12
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	2	0.12
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	4	0.12
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	9	0.12
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	2	0.12
(1,3138)	1:14:A:GLN:H	1:111:A:ARG:HD2	12	0.12
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	4	0.12
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	4	0.12
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	4	0.12
(1,3129)	1:18:A:ILE:HD11	1:66:A:ALA:HA	7	0.12
(1,3129)	1:18:A:ILE:HD12	1:66:A:ALA:HA	7	0.12
(1,3129)	1:18:A:ILE:HD13	1:66:A:ALA:HA	7	0.12
(1,3128)	1:85:A:MET:HE1	1:92:A:GLN:HE22	17	0.12
(1,3128)	1:85:A:MET:HE2	1:92:A:GLN:HE22	17	0.12
(1,3128)	1:85:A:MET:HE3	1:92:A:GLN:HE22	17	0.12
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD2	16	0.12
(1,3115)	1:37:A:ILE:H	1:53:A:LYS:HD3	16	0.12
(1,3103)	1:89:A:THR:H	1:92:A:GLN:HA	11	0.12
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	5	0.12
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	5	0.12
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	5	0.12
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	7	0.12
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	7	0.12
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	7	0.12
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	11	0.12
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	11	0.12
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	11	0.12
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	14	0.12
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	14	0.12
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	14	0.12
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	19	0.12
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	19	0.12
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	19	0.12
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	5	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	7	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	7	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	7	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	8	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	8	0.12
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	8	0.12
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	16	0.12
(1,3069)	1:74:A:GLY:H	1:112:A:GLN:HE22	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	1	0.12
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	20	0.12
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	3	0.12
(1,3034)	1:90:A:HIS:HB3	1:93:A:ALA:H	16	0.12
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	9	0.12
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	14	0.12
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	13	0.12
(1,3021)	1:115:A:GLN:HG2	1:117:A:ALA:H	8	0.12
(1,3021)	1:115:A:GLN:HG3	1:117:A:ALA:H	8	0.12
(1,3015)	1:89:A:THR:HG21	1:92:A:GLN:HE22	15	0.12
(1,3015)	1:89:A:THR:HG22	1:92:A:GLN:HE22	15	0.12
(1,3015)	1:89:A:THR:HG23	1:92:A:GLN:HE22	15	0.12
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE2	5	0.12
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE3	5	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD11	7	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD12	7	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD13	7	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD21	7	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD22	7	0.12
(1,2988)	1:14:A:GLN:HE21	1:107:A:LEU:HD23	7	0.12
(1,2984)	1:113:A:SER:HB2	1:115:A:GLN:H	11	0.12
(1,2984)	1:113:A:SER:HB3	1:115:A:GLN:H	11	0.12
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD2	16	0.12
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD3	16	0.12
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	12	0.12
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	18	0.12
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	10	0.12
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	10	0.12
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	1	0.12
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	12	0.12
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	16	0.12
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	16	0.12
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	16	0.12
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	16	0.12
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	16	0.12
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	16	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	18	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	18	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	18	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	18	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	18	0.12
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	18	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD11	3	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD12	3	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD13	3	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD21	3	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD22	3	0.12
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD23	3	0.12
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	12	0.12
(1,2817)	1:23:A:GLN:HB2	1:26:A:ASN:HD22	16	0.12
(1,2800)	1:20:A:LYS:HE2	1:22:A:ARG:H	18	0.12
(1,2800)	1:20:A:LYS:HE3	1:22:A:ARG:H	18	0.12
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	2	0.12
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	7	0.12
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	14	0.12
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	20	0.12
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	2	0.12
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	9	0.12
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	11	0.12
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	12	0.12
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	12	0.12
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	15	0.12
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	15	0.12
(1,2731)	1:118:A:VAL:HA	1:119:A:GLN:H	6	0.12
(1,2717)	1:116:A:LYS:H	1:116:A:LYS:HB3	8	0.12
(1,2670)	1:112:A:GLN:H	1:112:A:GLN:HB2	6	0.12
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	7	0.12
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	17	0.12
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	17	0.12
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	17	0.12
(1,2576)	1:98:A:THR:HA	1:100:A:ARG:H	19	0.12
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	4	0.12
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	4	0.12
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	13	0.12
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	13	0.12
(1,2538)	1:95:A:LYS:H	1:95:A:LYS:HB2	7	0.12
(1,2538)	1:95:A:LYS:H	1:95:A:LYS:HB2	9	0.12
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	15	0.12
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	1	0.12
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	3	0.12
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	6	0.12
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	14	0.12
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	18	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	11	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	11	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	11	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	16	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	16	0.12
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	16	0.12
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	15	0.12
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	15	0.12
(1,2316)	1:72:A:GLN:HB2	1:72:A:GLN:HE21	18	0.12
(1,2316)	1:72:A:GLN:HB3	1:72:A:GLN:HE21	18	0.12
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	10	0.12
(1,2229)	1:64:A:GLY:H	1:65:A:PRO:HD3	13	0.12
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	7	0.12
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	15	0.12
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	16	0.12
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG21	16	0.12
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG22	16	0.12
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG23	16	0.12
(1,2111)	1:51:A:THR:H	1:52:A:ASP:HB3	3	0.12
(1,1884)	1:29:A:LEU:HG	1:31:A:PHE:H	16	0.12
(1,1766)	1:16:A:VAL:HG21	1:17:A:GLU:H	20	0.12
(1,1766)	1:16:A:VAL:HG22	1:17:A:GLU:H	20	0.12
(1,1766)	1:16:A:VAL:HG23	1:17:A:GLU:H	20	0.12
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	13	0.12
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	14	0.12
(1,1710)	1:9:A:VAL:H	1:9:A:VAL:HB	18	0.12
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG21	19	0.12
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG22	19	0.12
(1,1675)	1:36:A:GLY:H	1:37:A:ILE:HG23	19	0.12
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	11	0.12
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	12	0.12
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	16	0.12
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	20	0.12
(1,1667)	1:14:A:GLN:HA	1:14:A:GLN:HE22	7	0.12
(1,1667)	1:14:A:GLN:HA	1:14:A:GLN:HE22	16	0.12
(1,1651)	1:78:A:MET:H	1:78:A:MET:HE1	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:78:A:MET:H	1:78:A:MET:HE2	20	0.12
(1,1651)	1:78:A:MET:H	1:78:A:MET:HE3	20	0.12
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	10	0.12
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	10	0.12
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	10	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	2	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	2	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	2	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	8	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	8	0.12
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	8	0.12
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE2	19	0.12
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE3	19	0.12
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	14	0.12
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	14	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB1	12	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB2	12	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB3	12	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB1	12	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB2	12	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB3	12	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB1	12	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB2	12	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB3	12	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB1	13	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB2	13	0.12
(1,1626)	1:16:A:VAL:HG11	1:66:A:ALA:HB3	13	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB1	13	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB2	13	0.12
(1,1626)	1:16:A:VAL:HG12	1:66:A:ALA:HB3	13	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB1	13	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB2	13	0.12
(1,1626)	1:16:A:VAL:HG13	1:66:A:ALA:HB3	13	0.12
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	7	0.12
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	7	0.12
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	10	0.12
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	10	0.12
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	1	0.12
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	1	0.12
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	1	0.12
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG11	18	0.12
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG12	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:85:A:MET:HB2	1:88:A:VAL:HG13	18	0.12
(1,1586)	1:83:A:TRP:HA	1:84:A:ASP:HB2	9	0.12
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB2	3	0.12
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB3	3	0.12
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	10	0.12
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	10	0.12
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	10	0.12
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	10	0.12
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	10	0.12
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	10	0.12
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	10	0.12
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	10	0.12
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	10	0.12
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	15	0.12
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	15	0.12
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	19	0.12
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	19	0.12
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	19	0.12
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	19	0.12
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	19	0.12
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	19	0.12
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	17	0.12
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	17	0.12
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	17	0.12
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	15	0.12
(1,1536)	1:13:A:VAL:HA	1:110:A:THR:HA	11	0.12
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG21	5	0.12
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG22	5	0.12
(1,1517)	1:19:A:HIS:HB3	1:104:A:VAL:HG23	5	0.12
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	2	0.12
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	9	0.12
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	10	0.12
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	16	0.12
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	4	0.12
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	4	0.12
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	4	0.12
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	6	0.12
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	6	0.12
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	6	0.12
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	10	0.12
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	10	0.12
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD11	17	0.12
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD12	17	0.12
(1,1464)	1:37:A:ILE:HG13	1:55:A:ILE:HD13	17	0.12
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	11	0.12
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	11	0.12
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	11	0.12
(1,1426)	1:13:A:VAL:HG21	1:14:A:GLN:H	13	0.12
(1,1426)	1:13:A:VAL:HG22	1:14:A:GLN:H	13	0.12
(1,1426)	1:13:A:VAL:HG23	1:14:A:GLN:H	13	0.12
(1,1424)	1:11:A:ALA:HB1	1:112:A:GLN:HB2	20	0.12
(1,1424)	1:11:A:ALA:HB2	1:112:A:GLN:HB2	20	0.12
(1,1424)	1:11:A:ALA:HB3	1:112:A:GLN:HB2	20	0.12
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	10	0.12
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	4	0.12
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	4	0.12
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	4	0.12
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	10	0.12
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	10	0.12
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	10	0.12
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	18	0.12
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	18	0.12
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	18	0.12
(1,1350)	1:33:A:ILE:HD11	1:94:A:ARG:HB3	2	0.12
(1,1350)	1:33:A:ILE:HD12	1:94:A:ARG:HB3	2	0.12
(1,1350)	1:33:A:ILE:HD13	1:94:A:ARG:HB3	2	0.12
(1,1350)	1:33:A:ILE:HD11	1:94:A:ARG:HB3	15	0.12
(1,1350)	1:33:A:ILE:HD12	1:94:A:ARG:HB3	15	0.12
(1,1350)	1:33:A:ILE:HD13	1:94:A:ARG:HB3	15	0.12
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	7	0.12
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	7	0.12
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	7	0.12
(1,1295)	1:91:A:ASP:H	1:91:A:ASP:HB2	17	0.12
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	3	0.12
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	2	0.12
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	2	0.12
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	2	0.12
(1,1227)	1:37:A:ILE:HD11	1:87:A:MET:HG3	19	0.12
(1,1227)	1:37:A:ILE:HD12	1:87:A:MET:HG3	19	0.12
(1,1227)	1:37:A:ILE:HD13	1:87:A:MET:HG3	19	0.12
(1,1118)	1:22:A:ARG:H	1:22:A:ARG:HD3	18	0.12
(1,1076)	1:116:A:LYS:HB2	1:117:A:ALA:H	10	0.12
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB2	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:112:A:GLN:HB3	1:113:A:SER:HB3	13	0.12
(1,1050)	1:112:A:GLN:HA	1:112:A:GLN:HG3	16	0.12
(1,1012)	1:110:A:THR:HA	1:111:A:ARG:HB2	17	0.12
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	15	0.12
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	15	0.12
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	15	0.12
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	18	0.12
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	18	0.12
(1,793)	1:65:A:PRO:HA	1:68:A:ILE:HG21	12	0.12
(1,793)	1:65:A:PRO:HA	1:68:A:ILE:HG22	12	0.12
(1,793)	1:65:A:PRO:HA	1:68:A:ILE:HG23	12	0.12
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	13	0.12
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	13	0.12
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	13	0.12
(1,725)	1:65:A:PRO:HB3	1:65:A:PRO:HD3	19	0.12
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	6	0.12
(1,682)	1:62:A:GLU:HG3	1:63:A:GLY:H	20	0.12
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	11	0.12
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	12	0.12
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	17	0.12
(1,670)	1:60:A:VAL:HG11	1:62:A:GLU:HA	7	0.12
(1,670)	1:60:A:VAL:HG12	1:62:A:GLU:HA	7	0.12
(1,670)	1:60:A:VAL:HG13	1:62:A:GLU:HA	7	0.12
(1,642)	1:60:A:VAL:HG11	1:61:A:SER:H	12	0.12
(1,642)	1:60:A:VAL:HG12	1:61:A:SER:H	12	0.12
(1,642)	1:60:A:VAL:HG13	1:61:A:SER:H	12	0.12
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB2	19	0.12
(1,560)	1:52:A:ASP:HB3	1:53:A:LYS:HB3	19	0.12
(1,551)	1:52:A:ASP:HA	1:53:A:LYS:H	13	0.12
(1,548)	1:51:A:THR:H	1:51:A:THR:HG21	6	0.12
(1,548)	1:51:A:THR:H	1:51:A:THR:HG22	6	0.12
(1,548)	1:51:A:THR:H	1:51:A:THR:HG23	6	0.12
(1,527)	1:95:A:LYS:HE2	1:99:A:LYS:HA	9	0.12
(1,527)	1:95:A:LYS:HE3	1:99:A:LYS:HA	9	0.12
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	20	0.12
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	9	0.12
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	9	0.12
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	9	0.12
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	14	0.12
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	14	0.12
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	14	0.12
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	4	0.12
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	6	0.12
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	9	0.12
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	10	0.12
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	18	0.12
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	12	0.12
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	12	0.12
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	12	0.12
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	11	0.12
(1,319)	1:32:A:SER:HB2	1:59:A:ARG:H	10	0.12
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	8	0.12
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	8	0.12
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	8	0.12
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	4	0.12
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	11	0.12
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	1	0.12
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	2	0.12
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	3	0.12
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	15	0.12
(1,257)	1:39:A:GLN:HG3	1:39:A:GLN:HE22	17	0.12
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	4	0.12
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	4	0.12
(1,217)	1:18:A:ILE:HD11	1:19:A:HIS:H	15	0.12
(1,217)	1:18:A:ILE:HD12	1:19:A:HIS:H	15	0.12
(1,217)	1:18:A:ILE:HD13	1:19:A:HIS:H	15	0.12
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	14	0.12
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	14	0.12
(1,128)	1:11:A:ALA:HB1	1:12:A:VAL:HA	8	0.12
(1,128)	1:11:A:ALA:HB2	1:12:A:VAL:HA	8	0.12
(1,128)	1:11:A:ALA:HB3	1:12:A:VAL:HA	8	0.12
(1,120)	1:10:A:THR:HG21	1:11:A:ALA:H	7	0.12
(1,120)	1:10:A:THR:HG22	1:11:A:ALA:H	7	0.12
(1,120)	1:10:A:THR:HG23	1:11:A:ALA:H	7	0.12
(1,71)	1:7:A:GLN:HA	1:8:A:PRO:HD2	11	0.12
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	14	0.11
(2,64)	1:59:A:ARG:O	1:73:A:ILE:N	18	0.11
(2,63)	1:59:A:ARG:N	1:73:A:ILE:O	15	0.11
(2,15)	1:92:A:GLN:O	1:96:A:ARG:H	3	0.11
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	15	0.11
(2,5)	1:16:A:VAL:H	1:107:A:LEU:O	6	0.11
(2,4)	1:14:A:GLN:O	1:109:A:VAL:H	9	0.11
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	2	0.11
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	2	0.11
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	5	0.11
(1,3180)	1:9:A:VAL:HA	1:11:A:ALA:H	17	0.11
(1,3179)	1:9:A:VAL:H	1:11:A:ALA:H	7	0.11
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	10	0.11
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	16	0.11
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	20	0.11
(1,3156)	1:36:A:GLY:H	1:55:A:ILE:H	15	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	6	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	6	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	6	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	6	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	6	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	6	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	6	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	6	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	6	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG21	16	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG22	16	0.11
(1,3153)	1:28:A:ILE:HD11	1:98:A:THR:HG23	16	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG21	16	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG22	16	0.11
(1,3153)	1:28:A:ILE:HD12	1:98:A:THR:HG23	16	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG21	16	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG22	16	0.11
(1,3153)	1:28:A:ILE:HD13	1:98:A:THR:HG23	16	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD11	4	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD12	4	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD13	4	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD21	4	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD22	4	0.11
(1,3149)	1:57:A:VAL:HG21	1:71:A:LEU:HD23	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD11	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD12	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD13	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD21	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD22	4	0.11
(1,3149)	1:57:A:VAL:HG22	1:71:A:LEU:HD23	4	0.11
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD11	4	0.11
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD12	4	0.11
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD13	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD21	4	0.11
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD22	4	0.11
(1,3149)	1:57:A:VAL:HG23	1:71:A:LEU:HD23	4	0.11
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	3	0.11
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	10	0.11
(1,3142)	1:29:A:LEU:HA	1:31:A:PHE:H	5	0.11
(1,3137)	1:14:A:GLN:H	1:111:A:ARG:HG3	12	0.11
(1,3133)	1:77:A:ILE:HB	1:110:A:THR:H	11	0.11
(1,3128)	1:85:A:MET:HE1	1:92:A:GLN:HE22	8	0.11
(1,3128)	1:85:A:MET:HE2	1:92:A:GLN:HE22	8	0.11
(1,3128)	1:85:A:MET:HE3	1:92:A:GLN:HE22	8	0.11
(1,3120)	1:72:A:GLN:HE21	1:115:A:GLN:HA	11	0.11
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD2	10	0.11
(1,3114)	1:36:A:GLY:H	1:53:A:LYS:HD3	10	0.11
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	12	0.11
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	12	0.11
(1,3106)	1:76:A:LYS:H	1:111:A:ARG:H	6	0.11
(1,3103)	1:89:A:THR:H	1:92:A:GLN:HA	7	0.11
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	2	0.11
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	2	0.11
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	2	0.11
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	6	0.11
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	6	0.11
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	6	0.11
(1,3098)	1:105:A:VAL:HG11	1:106:A:ARG:HB2	17	0.11
(1,3098)	1:105:A:VAL:HG12	1:106:A:ARG:HB2	17	0.11
(1,3098)	1:105:A:VAL:HG13	1:106:A:ARG:HB2	17	0.11
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	6	0.11
(1,3090)	1:4:A:ILE:HA	1:8:A:PRO:HD3	15	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	14	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	14	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	14	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB1	16	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB2	16	0.11
(1,3075)	1:88:A:VAL:H	1:93:A:ALA:HB3	16	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG21	16	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG22	16	0.11
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG23	16	0.11
(1,3059)	1:30:A:GLY:HA2	1:65:A:PRO:HG3	17	0.11
(1,3054)	1:77:A:ILE:HG21	1:79:A:GLN:HG2	5	0.11
(1,3054)	1:77:A:ILE:HG22	1:79:A:GLN:HG2	5	0.11
(1,3054)	1:77:A:ILE:HG23	1:79:A:GLN:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB1	8	0.11
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB2	8	0.11
(1,3053)	1:31:A:PHE:HB2	1:66:A:ALA:HB3	8	0.11
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	6	0.11
(1,3033)	1:83:A:TRP:HB3	1:83:A:TRP:HE1	9	0.11
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	4	0.11
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	5	0.11
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	10	0.11
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	5	0.11
(1,3030)	1:59:A:ARG:H	1:59:A:ARG:HG2	7	0.11
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	4	0.11
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	5	0.11
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	8	0.11
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	9	0.11
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	11	0.11
(1,3019)	1:19:A:HIS:HB2	1:105:A:VAL:H	4	0.11
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	7	0.11
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	7	0.11
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	19	0.11
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	19	0.11
(1,3013)	1:90:A:HIS:HB2	1:92:A:GLN:H	8	0.11
(1,3009)	1:83:A:TRP:HB3	1:83:A:TRP:HE1	9	0.11
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	14	0.11
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	14	0.11
(1,2981)	1:50:A:LYS:HD2	1:110:A:THR:H	12	0.11
(1,2981)	1:50:A:LYS:HD3	1:110:A:THR:H	12	0.11
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	7	0.11
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	8	0.11
(1,2974)	1:97:A:LEU:H	1:97:A:LEU:HG	15	0.11
(1,2974)	1:97:A:LEU:H	1:97:A:LEU:HG	19	0.11
(1,2972)	1:72:A:GLN:HB2	1:73:A:ILE:H	9	0.11
(1,2972)	1:72:A:GLN:HB3	1:73:A:ILE:H	9	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	3	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	3	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	3	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG21	20	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG22	20	0.11
(1,2969)	1:78:A:MET:H	1:110:A:THR:HG23	20	0.11
(1,2967)	1:33:A:ILE:HA	1:59:A:ARG:H	11	0.11
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	7	0.11
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	1	0.11
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	12	0.11
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	12	0.11
(1,2927)	1:20:A:LYS:HB2	1:104:A:VAL:H	17	0.11
(1,2927)	1:20:A:LYS:HB3	1:104:A:VAL:H	17	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	5	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	5	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	5	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG11	19	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG12	19	0.11
(1,2919)	1:85:A:MET:H	1:88:A:VAL:HG13	19	0.11
(1,2917)	1:80:A:VAL:HG11	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG12	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG13	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG21	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG22	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG23	1:84:A:ASP:H	1	0.11
(1,2917)	1:80:A:VAL:HG11	1:84:A:ASP:H	9	0.11
(1,2917)	1:80:A:VAL:HG12	1:84:A:ASP:H	9	0.11
(1,2917)	1:80:A:VAL:HG13	1:84:A:ASP:H	9	0.11
(1,2917)	1:80:A:VAL:HG21	1:84:A:ASP:H	9	0.11
(1,2917)	1:80:A:VAL:HG22	1:84:A:ASP:H	9	0.11
(1,2917)	1:80:A:VAL:HG23	1:84:A:ASP:H	9	0.11
(1,2912)	1:83:A:TRP:HE1	1:96:A:ARG:HB2	7	0.11
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	10	0.11
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	11	0.11
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	11	0.11
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	11	0.11
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	11	0.11
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	11	0.11
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	11	0.11
(1,2903)	1:79:A:GLN:HB2	1:83:A:TRP:H	15	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	3	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	3	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	3	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	3	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	3	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD11	17	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD12	17	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD13	17	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD21	17	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD22	17	0.11
(1,2901)	1:82:A:GLY:H	1:108:A:LEU:HD23	17	0.11
(1,2893)	1:81:A:ASN:HD22	1:106:A:ARG:HB3	18	0.11
(1,2873)	1:79:A:GLN:HE21	1:82:A:GLY:HA3	7	0.11
(1,2855)	1:57:A:VAL:HG21	1:75:A:ASP:H	19	0.11
(1,2855)	1:57:A:VAL:HG22	1:75:A:ASP:H	19	0.11
(1,2855)	1:57:A:VAL:HG23	1:75:A:ASP:H	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD11	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD12	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD13	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD21	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD22	19	0.11
(1,2832)	1:67:A:GLU:H	1:71:A:LEU:HD23	19	0.11
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	1	0.11
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	12	0.11
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	17	0.11
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	7	0.11
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	10	0.11
(1,2768)	1:12:A:VAL:H	1:110:A:THR:HB	15	0.11
(1,2705)	1:114:A:LEU:HD11	1:115:A:GLN:H	6	0.11
(1,2705)	1:114:A:LEU:HD12	1:115:A:GLN:H	6	0.11
(1,2705)	1:114:A:LEU:HD13	1:115:A:GLN:H	6	0.11
(1,2696)	1:112:A:GLN:HB3	1:114:A:LEU:H	1	0.11
(1,2695)	1:113:A:SER:H	1:114:A:LEU:HD21	15	0.11
(1,2695)	1:113:A:SER:H	1:114:A:LEU:HD22	15	0.11
(1,2695)	1:113:A:SER:H	1:114:A:LEU:HD23	15	0.11
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	1	0.11
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	10	0.11
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	11	0.11
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	18	0.11
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	20	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	5	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	5	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	5	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	13	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	13	0.11
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	13	0.11
(1,2586)	1:99:A:LYS:HG3	1:101:A:SER:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2559)	1:97:A:LEU:HG	1:98:A:THR:H	6	0.11
(1,2559)	1:97:A:LEU:HG	1:98:A:THR:H	16	0.11
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	2	0.11
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	2	0.11
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE2	3	0.11
(1,2539)	1:95:A:LYS:H	1:95:A:LYS:HE3	3	0.11
(1,2472)	1:55:A:ILE:HD11	1:91:A:ASP:H	3	0.11
(1,2472)	1:55:A:ILE:HD12	1:91:A:ASP:H	3	0.11
(1,2472)	1:55:A:ILE:HD13	1:91:A:ASP:H	3	0.11
(1,2469)	1:39:A:GLN:HG3	1:91:A:ASP:H	12	0.11
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	2	0.11
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	2	0.11
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG2	8	0.11
(1,2444)	1:89:A:THR:H	1:92:A:GLN:HG3	8	0.11
(1,2411)	1:84:A:ASP:H	1:84:A:ASP:HB2	2	0.11
(1,2411)	1:84:A:ASP:H	1:84:A:ASP:HB2	15	0.11
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	18	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	4	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	5	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	8	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	9	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	10	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	12	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	16	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	17	0.11
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	20	0.11
(1,2370)	1:79:A:GLN:HA	1:79:A:GLN:HE22	3	0.11
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG21	8	0.11
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG22	8	0.11
(1,2326)	1:73:A:ILE:H	1:73:A:ILE:HG23	8	0.11
(1,2323)	1:72:A:GLN:HG2	1:73:A:ILE:H	10	0.11
(1,2323)	1:72:A:GLN:HG3	1:73:A:ILE:H	10	0.11
(1,2321)	1:91:A:ASP:HB2	1:95:A:LYS:H	5	0.11
(1,2314)	1:71:A:LEU:HA	1:72:A:GLN:HE22	2	0.11
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	1	0.11
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	12	0.11
(1,2176)	1:32:A:SER:HB2	1:59:A:ARG:H	19	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG21	18	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG22	18	0.11
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG23	18	0.11
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE1	19	0.11
(1,2145)	1:55:A:ILE:H	1:56:A:TYR:HE2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2073)	1:46:A:PHE:HB3	1:47:A:SER:H	6	0.11
(1,2052)	1:44:A:ASN:H	1:45:A:PRO:HD2	19	0.11
(1,2031)	1:40:A:ASP:HB2	1:43:A:GLN:HE22	6	0.11
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	2	0.11
(1,2006)	1:39:A:GLN:HG3	1:40:A:ASP:H	18	0.11
(1,1987)	1:39:A:GLN:HE22	1:90:A:HIS:HA	15	0.11
(1,1985)	1:39:A:GLN:HE22	1:91:A:ASP:H	12	0.11
(1,1929)	1:35:A:GLY:H	1:90:A:HIS:HE1	7	0.11
(1,1929)	1:35:A:GLY:H	1:90:A:HIS:HE1	13	0.11
(1,1928)	1:35:A:GLY:H	1:90:A:HIS:HD2	12	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	13	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD11	15	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD12	15	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD13	15	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD21	15	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD22	15	0.11
(1,1874)	1:29:A:LEU:H	1:29:A:LEU:HD23	15	0.11
(1,1857)	1:27:A:LEU:H	1:27:A:LEU:HG	6	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD11	14	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD12	14	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD13	14	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD11	15	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD12	15	0.11
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD13	15	0.11
(1,1756)	1:15:A:ARG:H	1:15:A:ARG:HB2	20	0.11
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD2	3	0.11
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD3	3	0.11
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD2	11	0.11
(1,1728)	1:50:A:LYS:H	1:50:A:LYS:HD3	11	0.11
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	9	0.11
(1,1702)	1:4:A:ILE:H	1:7:A:GLN:HG2	16	0.11
(1,1702)	1:4:A:ILE:H	1:7:A:GLN:HG3	16	0.11
(1,1679)	1:114:A:LEU:HA	1:115:A:GLN:H	20	0.11
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	7	0.11
(1,1659)	1:72:A:GLN:HA	1:73:A:ILE:HG21	5	0.11
(1,1659)	1:72:A:GLN:HA	1:73:A:ILE:HG22	5	0.11
(1,1659)	1:72:A:GLN:HA	1:73:A:ILE:HG23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG2	16	0.11
(1,1655)	1:21:A:LEU:HA	1:22:A:ARG:HG3	16	0.11
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	4	0.11
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	4	0.11
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	7	0.11
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	7	0.11
(1,1654)	1:50:A:LYS:HB2	1:51:A:THR:HA	14	0.11
(1,1654)	1:50:A:LYS:HB3	1:51:A:THR:HA	14	0.11
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	6	0.11
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	6	0.11
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	6	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	13	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	13	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	13	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	15	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	15	0.11
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	15	0.11
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	17	0.11
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	17	0.11
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	18	0.11
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	18	0.11
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD2	10	0.11
(1,1629)	1:83:A:TRP:HB3	1:96:A:ARG:HD3	10	0.11
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	6	0.11
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	6	0.11
(1,1625)	1:50:A:LYS:HB2	1:51:A:THR:HB	14	0.11
(1,1625)	1:50:A:LYS:HB3	1:51:A:THR:HB	14	0.11
(1,1624)	1:46:A:PHE:H	1:47:A:SER:HB2	11	0.11
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	3	0.11
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	3	0.11
(1,1622)	1:23:A:GLN:HG2	1:25:A:GLU:H	16	0.11
(1,1622)	1:23:A:GLN:HG3	1:25:A:GLU:H	16	0.11
(1,1621)	1:18:A:ILE:HG21	1:65:A:PRO:HA	5	0.11
(1,1621)	1:18:A:ILE:HG22	1:65:A:PRO:HA	5	0.11
(1,1621)	1:18:A:ILE:HG23	1:65:A:PRO:HA	5	0.11
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	1	0.11
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	1	0.11
(1,1609)	1:17:A:GLU:HG3	1:19:A:HIS:HD2	14	0.11
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	16	0.11
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	16	0.11
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	16	0.11
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB3	1	0.11
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB2	12	0.11
(1,1579)	1:79:A:GLN:HB3	1:108:A:LEU:HB3	12	0.11
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	1	0.11
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	1	0.11
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	1	0.11
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	2	0.11
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	2	0.11
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	2	0.11
(1,1569)	1:78:A:MET:HE1	1:79:A:GLN:H	11	0.11
(1,1569)	1:78:A:MET:HE2	1:79:A:GLN:H	11	0.11
(1,1569)	1:78:A:MET:HE3	1:79:A:GLN:H	11	0.11
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG21	2	0.11
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG22	2	0.11
(1,1568)	1:78:A:MET:HE1	1:86:A:THR:HG23	2	0.11
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG21	2	0.11
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG22	2	0.11
(1,1568)	1:78:A:MET:HE2	1:86:A:THR:HG23	2	0.11
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG21	2	0.11
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG22	2	0.11
(1,1568)	1:78:A:MET:HE3	1:86:A:THR:HG23	2	0.11
(1,1567)	1:78:A:MET:HE1	1:86:A:THR:HA	20	0.11
(1,1567)	1:78:A:MET:HE2	1:86:A:THR:HA	20	0.11
(1,1567)	1:78:A:MET:HE3	1:86:A:THR:HA	20	0.11
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE1	11	0.11
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE2	11	0.11
(1,1565)	1:77:A:ILE:HD11	1:78:A:MET:HE3	11	0.11
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE1	11	0.11
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE2	11	0.11
(1,1565)	1:77:A:ILE:HD12	1:78:A:MET:HE3	11	0.11
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE1	11	0.11
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE2	11	0.11
(1,1565)	1:77:A:ILE:HD13	1:78:A:MET:HE3	11	0.11
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD11	11	0.11
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD12	11	0.11
(1,1564)	1:56:A:TYR:HD1	1:77:A:ILE:HD13	11	0.11
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD11	11	0.11
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD12	11	0.11
(1,1564)	1:56:A:TYR:HD2	1:77:A:ILE:HD13	11	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	1	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	1	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	1	0.11
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	1	0.11
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	1	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	14	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	14	0.11
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	14	0.11
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	14	0.11
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	14	0.11
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	14	0.11
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG21	3	0.11
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG22	3	0.11
(1,1545)	1:14:A:GLN:H	1:110:A:THR:HG23	3	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	3	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	3	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	3	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	3	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	3	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	3	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	3	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	3	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	3	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG21	8	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG22	8	0.11
(1,1544)	1:13:A:VAL:HG21	1:110:A:THR:HG23	8	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG21	8	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG22	8	0.11
(1,1544)	1:13:A:VAL:HG22	1:110:A:THR:HG23	8	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG21	8	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG22	8	0.11
(1,1544)	1:13:A:VAL:HG23	1:110:A:THR:HG23	8	0.11
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	2	0.11
(1,1541)	1:109:A:VAL:HA	1:110:A:THR:HB	17	0.11
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB2	18	0.11
(1,1474)	1:57:A:VAL:HG21	1:75:A:ASP:HB3	18	0.11
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB2	18	0.11
(1,1474)	1:57:A:VAL:HG22	1:75:A:ASP:HB3	18	0.11
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB2	18	0.11
(1,1474)	1:57:A:VAL:HG23	1:75:A:ASP:HB3	18	0.11
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	2	0.11
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	2	0.11
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	2	0.11
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	16	0.11
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	16	0.11
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	17	0.11
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	17	0.11
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	17	0.11
(1,1463)	1:44:A:ASN:H	1:45:A:PRO:HB3	19	0.11
(1,1450)	1:23:A:GLN:HB2	1:26:A:ASN:HB2	1	0.11
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG11	20	0.11
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG12	20	0.11
(1,1429)	1:14:A:GLN:HB3	1:109:A:VAL:HG13	20	0.11
(1,1426)	1:13:A:VAL:HG21	1:14:A:GLN:H	18	0.11
(1,1426)	1:13:A:VAL:HG22	1:14:A:GLN:H	18	0.11
(1,1426)	1:13:A:VAL:HG23	1:14:A:GLN:H	18	0.11
(1,1417)	1:7:A:GLN:HB3	1:8:A:PRO:HD3	1	0.11
(1,1400)	1:36:A:GLY:HA2	1:90:A:HIS:HD2	3	0.11
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	1	0.11
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	1	0.11
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	1	0.11
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	15	0.11
(1,1292)	1:91:A:ASP:HA	1:94:A:ARG:HG3	20	0.11
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG21	1	0.11
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG22	1	0.11
(1,1257)	1:37:A:ILE:HA	1:89:A:THR:HG23	1	0.11
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG21	16	0.11
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG22	16	0.11
(1,1216)	1:85:A:MET:H	1:86:A:THR:HG23	16	0.11
(1,1076)	1:116:A:LYS:HB2	1:117:A:ALA:H	8	0.11
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD21	14	0.11
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD22	14	0.11
(1,1065)	1:113:A:SER:HB2	1:114:A:LEU:HD23	14	0.11
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD21	14	0.11
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD22	14	0.11
(1,1065)	1:113:A:SER:HB3	1:114:A:LEU:HD23	14	0.11
(1,1045)	1:112:A:GLN:HG2	1:114:A:LEU:HD21	13	0.11
(1,1045)	1:112:A:GLN:HG2	1:114:A:LEU:HD22	13	0.11
(1,1045)	1:112:A:GLN:HG2	1:114:A:LEU:HD23	13	0.11
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD21	15	0.11
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD22	15	0.11
(1,1044)	1:112:A:GLN:HB3	1:114:A:LEU:HD23	15	0.11
(1,1024)	1:110:A:THR:HG21	1:112:A:GLN:HE21	17	0.11
(1,1024)	1:110:A:THR:HG22	1:112:A:GLN:HE21	17	0.11
(1,1024)	1:110:A:THR:HG23	1:112:A:GLN:HE21	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	19	0.11
(1,981)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	19	0.11
(1,981)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	19	0.11
(1,975)	1:105:A:VAL:HG11	1:106:A:ARG:HD3	18	0.11
(1,975)	1:105:A:VAL:HG12	1:106:A:ARG:HD3	18	0.11
(1,975)	1:105:A:VAL:HG13	1:106:A:ARG:HD3	18	0.11
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	8	0.11
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	8	0.11
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	8	0.11
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	13	0.11
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	13	0.11
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	13	0.11
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG11	16	0.11
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG12	16	0.11
(1,972)	1:20:A:LYS:HA	1:105:A:VAL:HG13	16	0.11
(1,916)	1:99:A:LYS:HA	1:100:A:ARG:HG3	3	0.11
(1,898)	1:95:A:LYS:HE2	1:99:A:LYS:HG2	8	0.11
(1,898)	1:95:A:LYS:HE3	1:99:A:LYS:HG2	8	0.11
(1,887)	1:97:A:LEU:HD11	1:98:A:THR:HA	12	0.11
(1,887)	1:97:A:LEU:HD12	1:98:A:THR:HA	12	0.11
(1,887)	1:97:A:LEU:HD13	1:98:A:THR:HA	12	0.11
(1,887)	1:97:A:LEU:HD21	1:98:A:THR:HA	12	0.11
(1,887)	1:97:A:LEU:HD22	1:98:A:THR:HA	12	0.11
(1,887)	1:97:A:LEU:HD23	1:98:A:THR:HA	12	0.11
(1,850)	1:95:A:LYS:HE2	1:99:A:LYS:HB3	20	0.11
(1,850)	1:95:A:LYS:HE3	1:99:A:LYS:HB3	20	0.11
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD11	11	0.11
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD12	11	0.11
(1,774)	1:65:A:PRO:HB2	1:68:A:ILE:HD13	11	0.11
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	4	0.11
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	4	0.11
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	4	0.11
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	6	0.11
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	6	0.11
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	6	0.11
(1,705)	1:65:A:PRO:HA	1:68:A:ILE:HG13	9	0.11
(1,679)	1:62:A:GLU:HA	1:62:A:GLU:HG3	11	0.11
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	3	0.11
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	6	0.11
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	7	0.11
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	8	0.11
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	19	0.11
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB1	16	0.11
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB2	16	0.11
(1,660)	1:61:A:SER:HB3	1:66:A:ALA:HB3	16	0.11
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	3	0.11
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	18	0.11
(1,629)	1:59:A:ARG:HG3	1:60:A:VAL:H	20	0.11
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD2	8	0.11
(1,619)	1:59:A:ARG:HA	1:59:A:ARG:HD3	8	0.11
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	17	0.11
(1,477)	1:44:A:ASN:HB2	1:45:A:PRO:HD2	7	0.11
(1,475)	1:44:A:ASN:H	1:45:A:PRO:HD2	19	0.11
(1,426)	1:40:A:ASP:HB3	1:41:A:PRO:HD2	2	0.11
(1,388)	1:37:A:ILE:HG21	1:88:A:VAL:H	2	0.11
(1,388)	1:37:A:ILE:HG22	1:88:A:VAL:H	2	0.11
(1,388)	1:37:A:ILE:HG23	1:88:A:VAL:H	2	0.11
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	18	0.11
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	18	0.11
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	18	0.11
(1,360)	1:36:A:GLY:HA3	1:55:A:ILE:HD11	8	0.11
(1,360)	1:36:A:GLY:HA3	1:55:A:ILE:HD12	8	0.11
(1,360)	1:36:A:GLY:HA3	1:55:A:ILE:HD13	8	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	1	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	7	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	8	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	11	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	13	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	15	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	16	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	17	0.11
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	20	0.11
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	16	0.11
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	16	0.11
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	16	0.11
(1,346)	1:33:A:ILE:HG21	1:90:A:HIS:HD2	20	0.11
(1,346)	1:33:A:ILE:HG22	1:90:A:HIS:HD2	20	0.11
(1,346)	1:33:A:ILE:HG23	1:90:A:HIS:HD2	20	0.11
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	18	0.11
(1,320)	1:32:A:SER:HB2	1:59:A:ARG:HA	6	0.11
(1,319)	1:32:A:SER:HB2	1:59:A:ARG:H	5	0.11
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	4	0.11
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	4	0.11
(1,281)	1:48:A:GLU:HG3	1:49:A:ASP:H	13	0.11
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	12	0.11
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	12	0.11
(1,235)	1:21:A:LEU:HA	1:22:A:ARG:HB3	2	0.11
(1,217)	1:18:A:ILE:HD11	1:19:A:HIS:H	13	0.11
(1,217)	1:18:A:ILE:HD12	1:19:A:HIS:H	13	0.11
(1,217)	1:18:A:ILE:HD13	1:19:A:HIS:H	13	0.11
(1,174)	1:15:A:ARG:H	1:15:A:ARG:HG2	10	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	7	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	7	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	10	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	10	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD2	17	0.11
(1,172)	1:15:A:ARG:H	1:15:A:ARG:HD3	17	0.11
(1,128)	1:11:A:ALA:HB1	1:12:A:VAL:HA	19	0.11
(1,128)	1:11:A:ALA:HB2	1:12:A:VAL:HA	19	0.11
(1,128)	1:11:A:ALA:HB3	1:12:A:VAL:HA	19	0.11
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	2	0.11
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	5	0.11
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	5	0.11
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	5	0.11
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	5	0.11
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	5	0.11
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	5	0.11
(1,86)	1:8:A:PRO:HG2	1:8:A:PRO:HA	6	0.11
(1,57)	1:8:A:PRO:HB2	1:8:A:PRO:HD3	9	0.11
(1,14)	1:15:A:ARG:HD2	1:16:A:VAL:HA	2	0.11
(1,14)	1:15:A:ARG:HD3	1:16:A:VAL:HA	2	0.11
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD11	11	0.11
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD12	11	0.11
(1,8)	1:63:A:GLY:HA3	1:68:A:ILE:HD13	11	0.11
(2,17)	1:94:A:ARG:O	1:98:A:THR:H	4	0.1
(2,17)	1:94:A:ARG:O	1:98:A:THR:H	11	0.1
(2,9)	1:21:A:LEU:H	1:28:A:ILE:O	7	0.1
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG11	5	0.1
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG12	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3185)	1:14:A:GLN:HB2	1:109:A:VAL:HG13	5	0.1
(1,3183)	1:13:A:VAL:HG21	1:110:A:THR:HB	14	0.1
(1,3183)	1:13:A:VAL:HG22	1:110:A:THR:HB	14	0.1
(1,3183)	1:13:A:VAL:HG23	1:110:A:THR:HB	14	0.1
(1,3164)	1:95:A:LYS:H	1:96:A:ARG:HA	19	0.1
(1,3154)	1:32:A:SER:HA	1:59:A:ARG:H	19	0.1
(1,3150)	1:29:A:LEU:HD11	1:99:A:LYS:H	13	0.1
(1,3150)	1:29:A:LEU:HD12	1:99:A:LYS:H	13	0.1
(1,3150)	1:29:A:LEU:HD13	1:99:A:LYS:H	13	0.1
(1,3150)	1:29:A:LEU:HD21	1:99:A:LYS:H	13	0.1
(1,3150)	1:29:A:LEU:HD22	1:99:A:LYS:H	13	0.1
(1,3150)	1:29:A:LEU:HD23	1:99:A:LYS:H	13	0.1
(1,3143)	1:36:A:GLY:H	1:54:A:GLY:H	6	0.1
(1,3109)	1:56:A:TYR:HD1	1:76:A:LYS:H	11	0.1
(1,3109)	1:56:A:TYR:HD2	1:76:A:LYS:H	11	0.1
(1,3094)	1:24:A:GLY:H	1:25:A:GLU:HG3	2	0.1
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG21	7	0.1
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG22	7	0.1
(1,3073)	1:56:A:TYR:HA	1:77:A:ILE:HG23	7	0.1
(1,3038)	1:35:A:GLY:HA2	1:39:A:GLN:H	15	0.1
(1,3032)	1:57:A:VAL:HB	1:75:A:ASP:H	19	0.1
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	2	0.1
(1,3031)	1:65:A:PRO:HB3	1:66:A:ALA:H	11	0.1
(1,3028)	1:78:A:MET:HA	1:86:A:THR:H	18	0.1
(1,3016)	1:20:A:LYS:HB2	1:101:A:SER:H	8	0.1
(1,3016)	1:20:A:LYS:HB3	1:101:A:SER:H	8	0.1
(1,3015)	1:89:A:THR:HG21	1:92:A:GLN:HE22	19	0.1
(1,3015)	1:89:A:THR:HG22	1:92:A:GLN:HE22	19	0.1
(1,3015)	1:89:A:THR:HG23	1:92:A:GLN:HE22	19	0.1
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE2	12	0.1
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE3	12	0.1
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE2	13	0.1
(1,3008)	1:83:A:TRP:HE1	1:95:A:LYS:HE3	13	0.1
(1,3000)	1:47:A:SER:H	1:49:A:ASP:H	12	0.1
(1,2999)	1:47:A:SER:H	1:49:A:ASP:H	12	0.1
(1,2981)	1:50:A:LYS:HD2	1:110:A:THR:H	2	0.1
(1,2981)	1:50:A:LYS:HD3	1:110:A:THR:H	2	0.1
(1,2978)	1:112:A:GLN:HA	1:113:A:SER:H	12	0.1
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD2	20	0.1
(1,2973)	1:95:A:LYS:H	1:95:A:LYS:HD3	20	0.1
(1,2963)	1:13:A:VAL:HB	1:14:A:GLN:H	3	0.1
(1,2961)	1:24:A:GLY:HA2	1:26:A:ASN:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG11	20	0.1
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG12	20	0.1
(1,2921)	1:86:A:THR:H	1:88:A:VAL:HG13	20	0.1
(1,2917)	1:80:A:VAL:HG11	1:84:A:ASP:H	3	0.1
(1,2917)	1:80:A:VAL:HG12	1:84:A:ASP:H	3	0.1
(1,2917)	1:80:A:VAL:HG13	1:84:A:ASP:H	3	0.1
(1,2917)	1:80:A:VAL:HG21	1:84:A:ASP:H	3	0.1
(1,2917)	1:80:A:VAL:HG22	1:84:A:ASP:H	3	0.1
(1,2917)	1:80:A:VAL:HG23	1:84:A:ASP:H	3	0.1
(1,2916)	1:79:A:GLN:HG3	1:84:A:ASP:H	6	0.1
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE1	10	0.1
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE2	10	0.1
(1,2910)	1:83:A:TRP:HE1	1:85:A:MET:HE3	10	0.1
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	9	0.1
(1,2908)	1:80:A:VAL:HG11	1:83:A:TRP:HE1	19	0.1
(1,2908)	1:80:A:VAL:HG12	1:83:A:TRP:HE1	19	0.1
(1,2908)	1:80:A:VAL:HG13	1:83:A:TRP:HE1	19	0.1
(1,2908)	1:80:A:VAL:HG21	1:83:A:TRP:HE1	19	0.1
(1,2908)	1:80:A:VAL:HG22	1:83:A:TRP:HE1	19	0.1
(1,2908)	1:80:A:VAL:HG23	1:83:A:TRP:HE1	19	0.1
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD2	6	0.1
(1,2907)	1:83:A:TRP:HE1	1:95:A:LYS:HD3	6	0.1
(1,2798)	1:20:A:LYS:HA	1:22:A:ARG:H	13	0.1
(1,2794)	1:21:A:LEU:H	1:27:A:LEU:HG	15	0.1
(1,2763)	1:78:A:MET:HG2	1:108:A:LEU:H	7	0.1
(1,2763)	1:78:A:MET:HG3	1:108:A:LEU:H	7	0.1
(1,2762)	1:82:A:GLY:H	1:106:A:ARG:H	3	0.1
(1,2719)	1:116:A:LYS:H	1:118:A:VAL:HB	4	0.1
(1,2654)	1:109:A:VAL:HB	1:110:A:THR:H	19	0.1
(1,2652)	1:50:A:LYS:HG2	1:110:A:THR:H	3	0.1
(1,2652)	1:50:A:LYS:HG3	1:110:A:THR:H	3	0.1
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG21	18	0.1
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG22	18	0.1
(1,2644)	1:109:A:VAL:H	1:109:A:VAL:HG23	18	0.1
(1,2601)	1:102:A:GLU:H	1:102:A:GLU:HG2	2	0.1
(1,2516)	1:93:A:ALA:H	1:94:A:ARG:HB3	8	0.1
(1,2509)	1:91:A:ASP:HB2	1:93:A:ALA:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2452)	1:36:A:GLY:HA2	1:90:A:HIS:H	5	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	1	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	1	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	1	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG21	6	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG22	6	0.1
(1,2441)	1:88:A:VAL:H	1:88:A:VAL:HG23	6	0.1
(1,2407)	1:83:A:TRP:HD1	1:84:A:ASP:H	4	0.1
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	2	0.1
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	7	0.1
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	13	0.1
(1,2404)	1:83:A:TRP:HH2	1:83:A:TRP:HE1	19	0.1
(1,2402)	1:83:A:TRP:HA	1:83:A:TRP:HE1	13	0.1
(1,2374)	1:79:A:GLN:HE22	1:80:A:VAL:H	16	0.1
(1,2314)	1:71:A:LEU:HA	1:72:A:GLN:HE22	6	0.1
(1,2314)	1:71:A:LEU:HA	1:72:A:GLN:HE22	19	0.1
(1,2222)	1:63:A:GLY:H	1:68:A:ILE:H	2	0.1
(1,2180)	1:59:A:ARG:H	1:59:A:ARG:HG3	14	0.1
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG21	3	0.1
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG22	3	0.1
(1,2165)	1:57:A:VAL:H	1:57:A:VAL:HG23	3	0.1
(1,2122)	1:52:A:ASP:HB2	1:53:A:LYS:H	18	0.1
(1,2043)	1:41:A:PRO:HA	1:44:A:ASN:H	14	0.1
(1,1985)	1:39:A:GLN:HE22	1:91:A:ASP:H	5	0.1
(1,1929)	1:35:A:GLY:H	1:90:A:HIS:HE1	15	0.1
(1,1929)	1:35:A:GLY:H	1:90:A:HIS:HE1	17	0.1
(1,1928)	1:35:A:GLY:H	1:90:A:HIS:HD2	5	0.1
(1,1922)	1:34:A:GLY:HA3	1:35:A:GLY:H	4	0.1
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD11	16	0.1
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD12	16	0.1
(1,1775)	1:18:A:ILE:H	1:18:A:ILE:HD13	16	0.1
(1,1753)	1:14:A:GLN:HG2	1:15:A:ARG:H	4	0.1
(1,1722)	1:11:A:ALA:H	1:12:A:VAL:H	7	0.1
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	5	0.1
(1,1670)	1:25:A:GLU:HA	1:26:A:ASN:HD22	8	0.1
(1,1646)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	9	0.1
(1,1646)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	9	0.1
(1,1646)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	9	0.1
(1,1645)	1:65:A:PRO:HB2	1:68:A:ILE:H	6	0.1
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	14	0.1
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	14	0.1
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB1	18	0.1
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB2	18	0.1
(1,1641)	1:10:A:THR:HA	1:11:A:ALA:HB3	18	0.1
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE2	18	0.1
(1,1634)	1:52:A:ASP:HA	1:53:A:LYS:HE3	18	0.1
(1,1631)	1:98:A:THR:HG21	1:100:A:ARG:HA	12	0.1
(1,1631)	1:98:A:THR:HG22	1:100:A:ARG:HA	12	0.1
(1,1631)	1:98:A:THR:HG23	1:100:A:ARG:HA	12	0.1
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE2	16	0.1
(1,1630)	1:98:A:THR:HA	1:99:A:LYS:HE3	16	0.1
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE1	4	0.1
(1,1616)	1:55:A:ILE:HG13	1:56:A:TYR:HE2	4	0.1
(1,1609)	1:17:A:GLU:HG3	1:19:A:HIS:HD2	2	0.1
(1,1609)	1:17:A:GLU:HG3	1:19:A:HIS:HD2	9	0.1
(1,1609)	1:17:A:GLU:HG3	1:19:A:HIS:HD2	10	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	11	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	11	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	11	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE1	19	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE2	19	0.1
(1,1597)	1:84:A:ASP:HA	1:85:A:MET:HE3	19	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD11	20	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD12	20	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD13	20	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD21	20	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD22	20	0.1
(1,1566)	1:78:A:MET:HB3	1:108:A:LEU:HD23	20	0.1
(1,1555)	1:11:A:ALA:HB1	1:112:A:GLN:HG2	16	0.1
(1,1555)	1:11:A:ALA:HB2	1:112:A:GLN:HG2	16	0.1
(1,1555)	1:11:A:ALA:HB3	1:112:A:GLN:HG2	16	0.1
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB2	9	0.1
(1,1554)	1:112:A:GLN:HA	1:113:A:SER:HB3	9	0.1
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG21	8	0.1
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG22	8	0.1
(1,1547)	1:78:A:MET:HG2	1:110:A:THR:HG23	8	0.1
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG21	8	0.1
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG22	8	0.1
(1,1547)	1:78:A:MET:HG3	1:110:A:THR:HG23	8	0.1
(1,1537)	1:13:A:VAL:HG21	1:110:A:THR:HA	5	0.1
(1,1537)	1:13:A:VAL:HG22	1:110:A:THR:HA	5	0.1
(1,1537)	1:13:A:VAL:HG23	1:110:A:THR:HA	5	0.1
(1,1512)	1:80:A:VAL:HG11	1:96:A:ARG:HD2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1512)	1:80:A:VAL:HG11	1:96:A:ARG:HD3	10	0.1
(1,1512)	1:80:A:VAL:HG12	1:96:A:ARG:HD2	10	0.1
(1,1512)	1:80:A:VAL:HG12	1:96:A:ARG:HD3	10	0.1
(1,1512)	1:80:A:VAL:HG13	1:96:A:ARG:HD2	10	0.1
(1,1512)	1:80:A:VAL:HG13	1:96:A:ARG:HD3	10	0.1
(1,1512)	1:80:A:VAL:HG21	1:96:A:ARG:HD2	10	0.1
(1,1512)	1:80:A:VAL:HG21	1:96:A:ARG:HD3	10	0.1
(1,1512)	1:80:A:VAL:HG22	1:96:A:ARG:HD2	10	0.1
(1,1512)	1:80:A:VAL:HG22	1:96:A:ARG:HD3	10	0.1
(1,1512)	1:80:A:VAL:HG23	1:96:A:ARG:HD2	10	0.1
(1,1512)	1:80:A:VAL:HG23	1:96:A:ARG:HD3	10	0.1
(1,1510)	1:94:A:ARG:HB3	1:95:A:LYS:HA	15	0.1
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD11	14	0.1
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD12	14	0.1
(1,1504)	1:60:A:VAL:HG11	1:73:A:ILE:HD13	14	0.1
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD11	14	0.1
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD12	14	0.1
(1,1504)	1:60:A:VAL:HG12	1:73:A:ILE:HD13	14	0.1
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD11	14	0.1
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD12	14	0.1
(1,1504)	1:60:A:VAL:HG13	1:73:A:ILE:HD13	14	0.1
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	5	0.1
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	5	0.1
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	5	0.1
(1,1475)	1:58:A:THR:HG21	1:59:A:ARG:H	17	0.1
(1,1475)	1:58:A:THR:HG22	1:59:A:ARG:H	17	0.1
(1,1475)	1:58:A:THR:HG23	1:59:A:ARG:H	17	0.1
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	4	0.1
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	4	0.1
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	4	0.1
(1,1472)	1:57:A:VAL:HG11	1:75:A:ASP:H	14	0.1
(1,1472)	1:57:A:VAL:HG12	1:75:A:ASP:H	14	0.1
(1,1472)	1:57:A:VAL:HG13	1:75:A:ASP:H	14	0.1
(1,1426)	1:13:A:VAL:HG21	1:14:A:GLN:H	1	0.1
(1,1426)	1:13:A:VAL:HG22	1:14:A:GLN:H	1	0.1
(1,1426)	1:13:A:VAL:HG23	1:14:A:GLN:H	1	0.1
(1,1421)	1:8:A:PRO:HD2	1:10:A:THR:HG21	4	0.1
(1,1421)	1:8:A:PRO:HD2	1:10:A:THR:HG22	4	0.1
(1,1421)	1:8:A:PRO:HD2	1:10:A:THR:HG23	4	0.1
(1,1404)	1:33:A:ILE:HD11	1:90:A:HIS:HE1	4	0.1
(1,1404)	1:33:A:ILE:HD12	1:90:A:HIS:HE1	4	0.1
(1,1404)	1:33:A:ILE:HD13	1:90:A:HIS:HE1	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:33:A:ILE:HD11	1:94:A:ARG:HG2	20	0.1
(1,1357)	1:33:A:ILE:HD12	1:94:A:ARG:HG2	20	0.1
(1,1357)	1:33:A:ILE:HD13	1:94:A:ARG:HG2	20	0.1
(1,1341)	1:91:A:ASP:HA	1:94:A:ARG:HA	8	0.1
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB1	3	0.1
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB2	3	0.1
(1,1320)	1:92:A:GLN:HB2	1:93:A:ALA:HB3	3	0.1
(1,1309)	1:88:A:VAL:HA	1:92:A:GLN:HB2	2	0.1
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	3	0.1
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	3	0.1
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	3	0.1
(1,1219)	1:86:A:THR:HG21	1:87:A:MET:HG2	7	0.1
(1,1219)	1:86:A:THR:HG22	1:87:A:MET:HG2	7	0.1
(1,1219)	1:86:A:THR:HG23	1:87:A:MET:HG2	7	0.1
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD21	6	0.1
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD22	6	0.1
(1,1060)	1:113:A:SER:HA	1:114:A:LEU:HD23	6	0.1
(1,981)	1:105:A:VAL:HG21	1:106:A:ARG:HD2	18	0.1
(1,981)	1:105:A:VAL:HG22	1:106:A:ARG:HD2	18	0.1
(1,981)	1:105:A:VAL:HG23	1:106:A:ARG:HD2	18	0.1
(1,974)	1:105:A:VAL:HG11	1:106:A:ARG:HD2	20	0.1
(1,974)	1:105:A:VAL:HG12	1:106:A:ARG:HD2	20	0.1
(1,974)	1:105:A:VAL:HG13	1:106:A:ARG:HD2	20	0.1
(1,887)	1:97:A:LEU:HD11	1:98:A:THR:HA	8	0.1
(1,887)	1:97:A:LEU:HD12	1:98:A:THR:HA	8	0.1
(1,887)	1:97:A:LEU:HD13	1:98:A:THR:HA	8	0.1
(1,887)	1:97:A:LEU:HD21	1:98:A:THR:HA	8	0.1
(1,887)	1:97:A:LEU:HD22	1:98:A:THR:HA	8	0.1
(1,887)	1:97:A:LEU:HD23	1:98:A:THR:HA	8	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	3	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	3	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	3	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG21	7	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG22	7	0.1
(1,832)	1:73:A:ILE:H	1:73:A:ILE:HG23	7	0.1
(1,828)	1:73:A:ILE:H	1:73:A:ILE:HG12	12	0.1
(1,729)	1:28:A:ILE:HG21	1:65:A:PRO:HG2	14	0.1
(1,729)	1:28:A:ILE:HG22	1:65:A:PRO:HG2	14	0.1
(1,729)	1:28:A:ILE:HG23	1:65:A:PRO:HG2	14	0.1
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	1	0.1
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	5	0.1
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:62:A:GLU:HA	1:63:A:GLY:HA3	15	0.1
(1,658)	1:61:A:SER:HA	1:62:A:GLU:HB2	7	0.1
(1,559)	1:52:A:ASP:HB2	1:53:A:LYS:H	18	0.1
(1,522)	1:47:A:SER:HB2	1:49:A:ASP:H	12	0.1
(1,504)	1:47:A:SER:HA	1:52:A:ASP:HB2	15	0.1
(1,502)	1:45:A:PRO:HG3	1:46:A:PHE:H	7	0.1
(1,369)	1:37:A:ILE:HD11	1:38:A:ASP:HA	11	0.1
(1,369)	1:37:A:ILE:HD12	1:38:A:ASP:HA	11	0.1
(1,369)	1:37:A:ILE:HD13	1:38:A:ASP:HA	11	0.1
(1,349)	1:34:A:GLY:HA3	1:35:A:GLY:H	14	0.1
(1,321)	1:32:A:SER:HB3	1:59:A:ARG:HA	16	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	13	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	13	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	13	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG21	17	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG22	17	0.1
(1,318)	1:32:A:SER:HB2	1:33:A:ILE:HG23	17	0.1
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG2	2	0.1
(1,252)	1:23:A:GLN:H	1:23:A:GLN:HG3	2	0.1
(1,217)	1:18:A:ILE:HD11	1:19:A:HIS:H	14	0.1
(1,217)	1:18:A:ILE:HD12	1:19:A:HIS:H	14	0.1
(1,217)	1:18:A:ILE:HD13	1:19:A:HIS:H	14	0.1
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD2	11	0.1
(1,171)	1:14:A:GLN:HE22	1:15:A:ARG:HD3	11	0.1
(1,114)	1:9:A:VAL:HG11	1:10:A:THR:HB	17	0.1
(1,114)	1:9:A:VAL:HG12	1:10:A:THR:HB	17	0.1
(1,114)	1:9:A:VAL:HG13	1:10:A:THR:HB	17	0.1
(1,114)	1:9:A:VAL:HG21	1:10:A:THR:HB	17	0.1
(1,114)	1:9:A:VAL:HG22	1:10:A:THR:HB	17	0.1
(1,114)	1:9:A:VAL:HG23	1:10:A:THR:HB	17	0.1
(1,4)	1:22:A:ARG:HD2	1:23:A:GLN:H	8	0.1

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

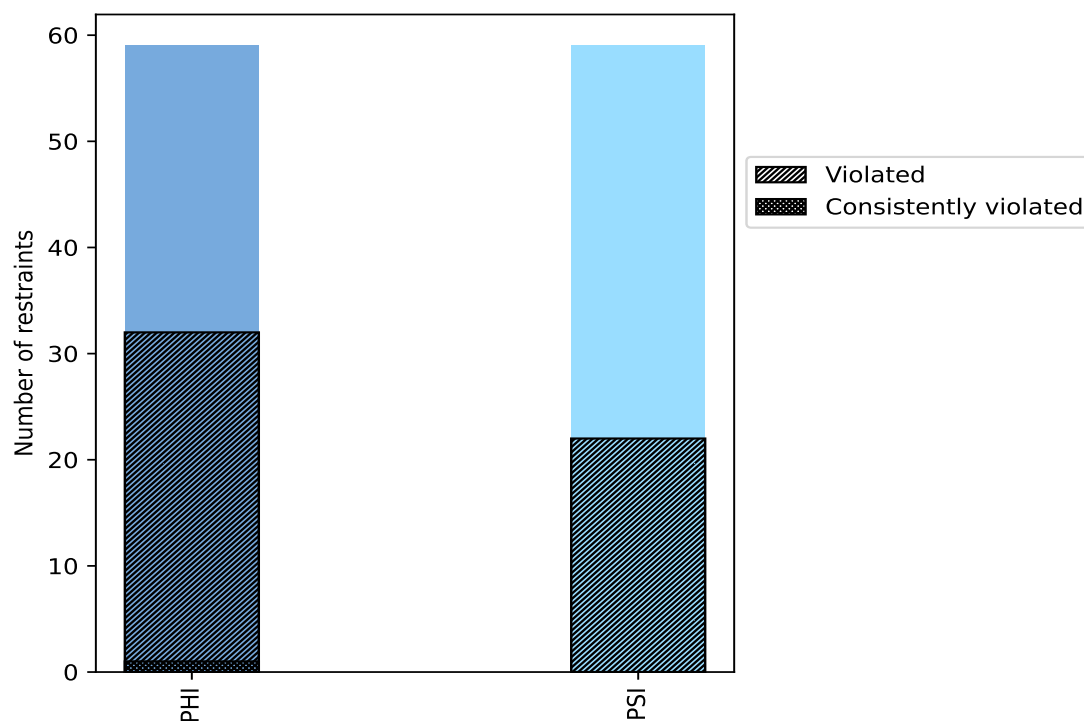
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	59	50.0	32	54.2	27.1	1	1.7	0.8
PSI	59	50.0	22	37.3	18.6	0	0.0	0.0
Total	118	100.0	54	45.8	45.8	1	0.8	0.8

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

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



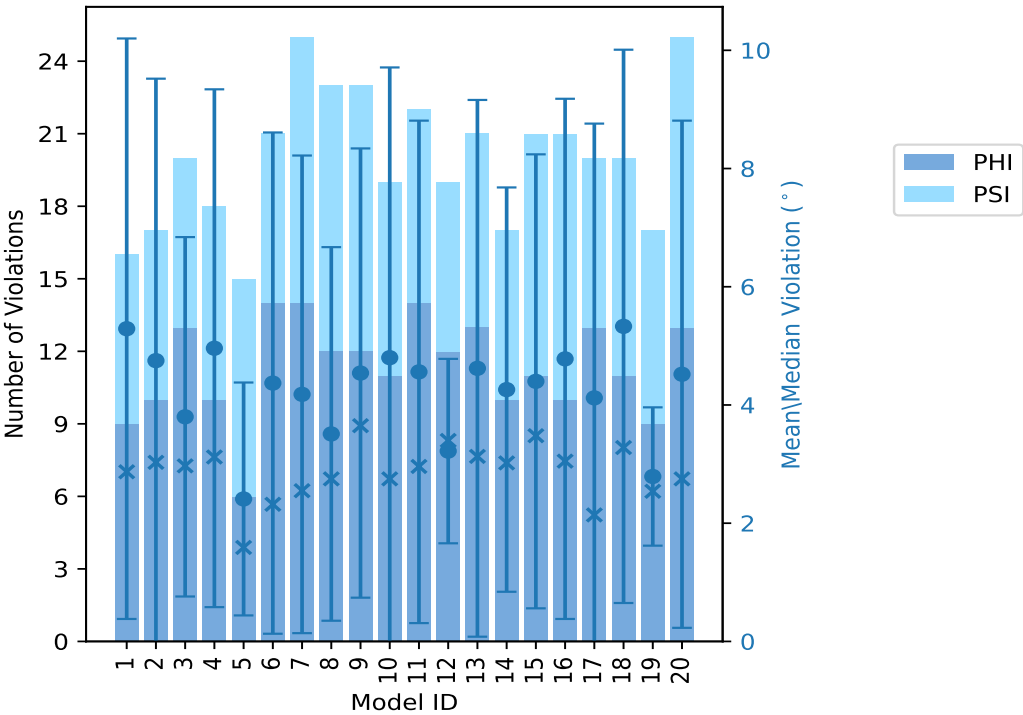
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	9	7	16	5.29	17.82	4.91	2.87
2	10	7	17	4.75	17.1	4.77	3.03
3	13	7	20	3.8	14.25	3.04	2.97
4	10	8	18	4.96	16.16	4.38	3.12
5	6	9	15	2.41	7.74	1.97	1.59
6	14	7	21	4.37	16.05	4.24	2.32
7	14	11	25	4.18	16.02	4.04	2.55
8	12	11	23	3.51	15.6	3.16	2.75
9	12	11	23	4.54	16.64	3.8	3.65
10	11	8	19	4.8	18.48	4.91	2.75
11	14	8	22	4.56	15.65	4.25	2.96
12	12	7	19	3.22	6.9	1.56	3.4
13	13	8	21	4.62	18.55	4.54	3.13
14	10	7	17	4.26	13.89	3.42	3.02
15	11	10	21	4.4	14.97	3.84	3.48
16	10	11	21	4.78	17.62	4.4	3.05
17	13	7	20	4.12	17.29	4.64	2.14
18	11	9	20	5.33	18.29	4.68	3.28
19	9	8	17	2.79	4.9	1.17	2.54
20	13	12	25	4.52	17.35	4.29	2.75

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
6	3	9	1	5.0
6	2	8	2	10.0
2	1	3	3	15.0
3	3	6	4	20.0
1	3	4	5	25.0
1	1	2	6	30.0
0	1	1	7	35.0
2	0	2	8	40.0
1	2	3	9	45.0
1	0	1	10	50.0
2	0	2	11	55.0

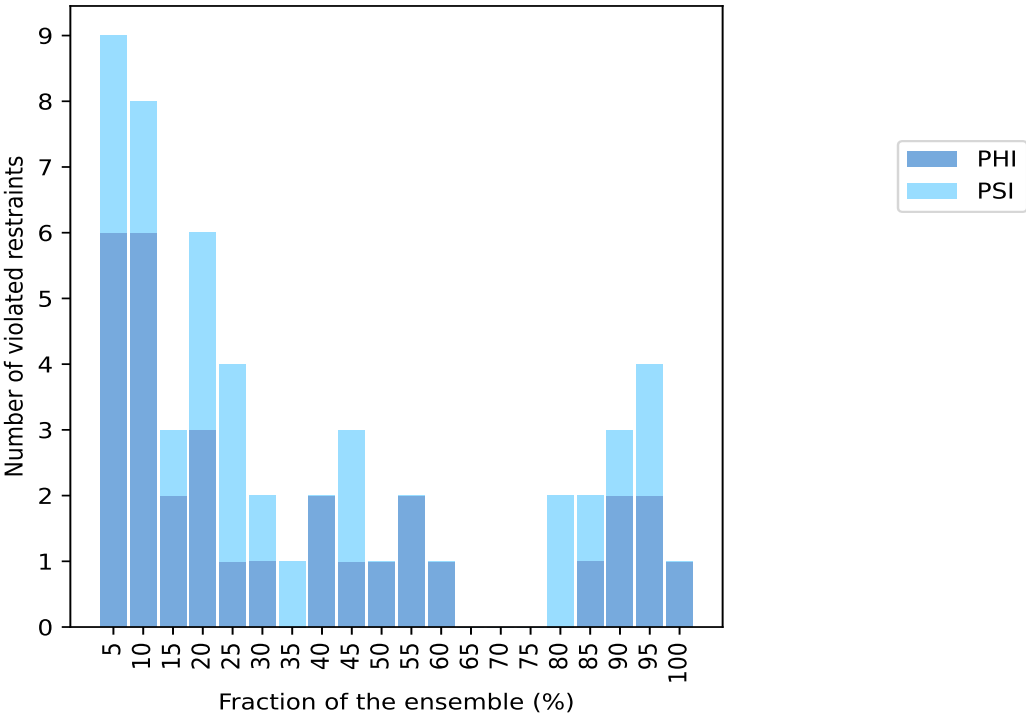
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	0	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	2	2	16	80.0
1	1	2	17	85.0
2	1	3	18	90.0
2	2	4	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

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

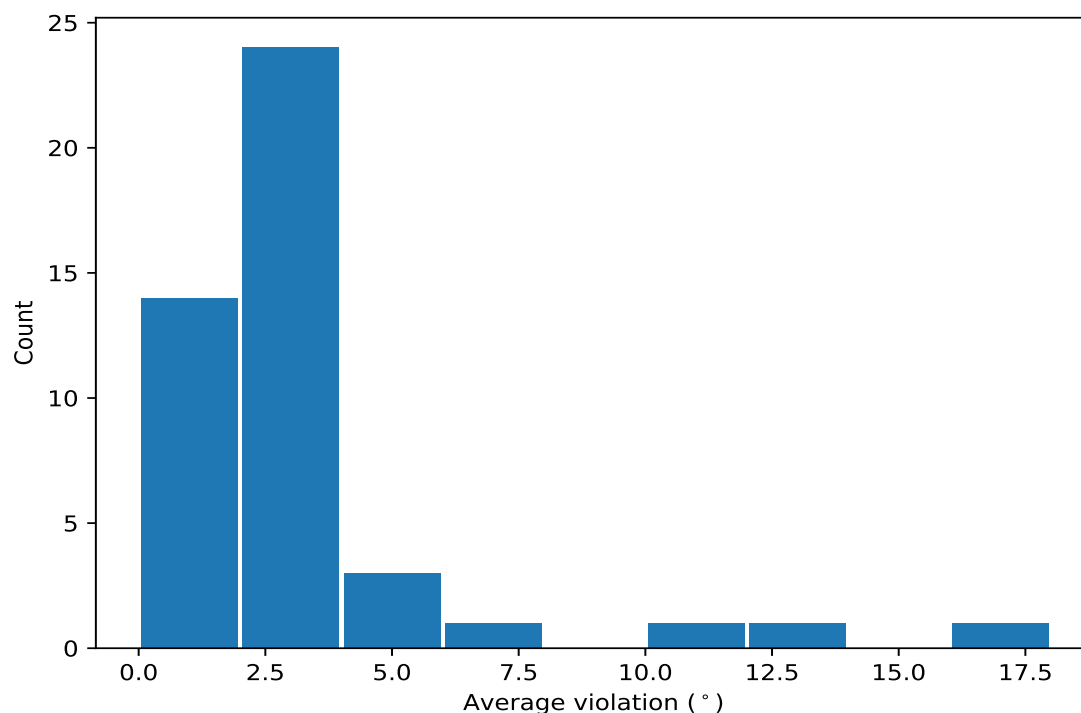


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	20	5.46	0.96	5.3
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	19	12.32	5.15	15.19
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	19	3.91	1.43	3.9
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	19	3.75	1.43	3.75
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	19	2.83	0.82	2.71
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	18	3.32	1.46	3.04
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	18	2.97	0.89	2.96
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	18	2.41	1.14	1.96
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	17	16.38	1.47	16.16
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	17	10.53	0.71	10.66
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	16	2.43	0.84	2.32
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	16	2.28	1.03	2.02
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	12	2.95	1.08	2.83
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	11	2.96	1.36	2.64
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	11	2.22	1.1	1.8
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	10	3.88	1.66	4.49
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	9	2.75	1.01	2.79
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	9	2.59	1.18	2.47
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	9	1.62	0.29	1.55
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	8	6.54	2.47	7.79

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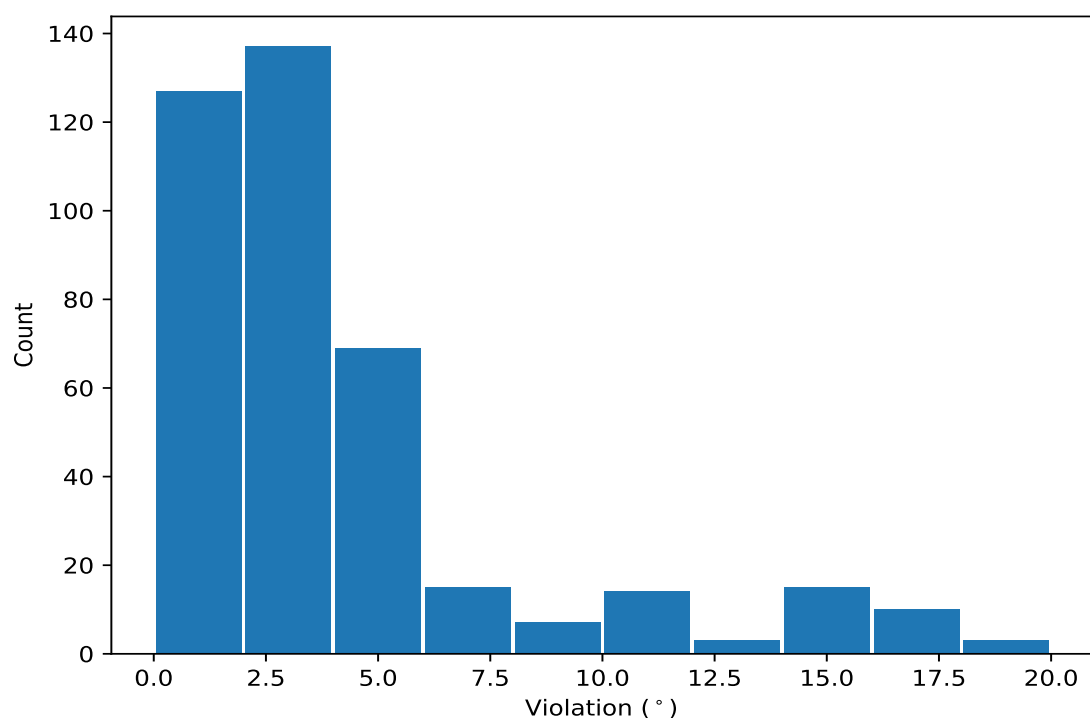
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	8	3.53	2.02	2.98
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	7	4.04	3.0	3.92
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	6	2.23	1.1	1.86
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	6	1.94	0.58	1.74
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	5	2.07	0.77	1.77
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	5	1.89	0.58	1.71
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	5	1.56	0.53	1.35
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	5	1.46	0.25	1.48
(1,93)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:LYS:N	4	2.9	1.24	2.5
(1,101)	1:84:A:ASP:N	1:84:A:ASP:CA	1:84:A:ASP:C	1:85:A:MET:N	4	2.08	1.16	1.64
(1,26)	1:55:A:ILE:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	4	2.03	0.6	2.18
(1,86)	1:59:A:ARG:N	1:59:A:ARG:CA	1:59:A:ARG:C	1:60:A:VAL:N	4	1.9	0.54	1.76
(1,8)	1:16:A:VAL:C	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	4	1.4	0.39	1.31
(1,45)	1:90:A:HIS:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	4	1.37	0.21	1.39
(1,52)	1:103:A:GLU:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	3	4.53	2.61	4.8
(1,82)	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	1:49:A:ASP:N	3	2.08	1.23	1.21
(1,20)	1:33:A:ILE:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	3	1.37	0.26	1.46
(1,30)	1:59:A:ARG:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	2	3.04	0.5	3.04
(1,77)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ILE:N	2	2.78	0.38	2.78
(1,56)	1:107:A:LEU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	2	2.12	0.93	2.12
(1,59)	1:110:A:THR:C	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	2	1.99	0.23	1.99
(1,47)	1:92:A:GLN:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	2	1.9	0.72	1.9
(1,105)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:ALA:N	2	1.77	0.21	1.77
(1,9)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	2	1.49	0.18	1.49
(1,35)	1:75:A:ASP:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	2	1.23	0.12	1.23

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 (°)
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	13	18.55
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	10	18.48
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	18	18.29
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1	17.82
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	16	17.62
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	20	17.35
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	17	17.29
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	2	17.1
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	9	16.64
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	4	16.16
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	10	16.09
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	6	16.05
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	7	16.02
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	17	15.79
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	20	15.79
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	11	15.65
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	8	15.6
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	4	15.51
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	11	15.5
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	16	15.4
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	18	15.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	2	15.28
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1	15.19
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	13	15.18
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	7	15.09
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	15	14.97
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	15	14.57
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	3	14.25
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	6	13.91
(1,21)	1:34:A:GLY:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	14	13.89
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	9	12.65
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	16	11.7
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	10	11.5
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	13	11.11
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	9	11.1
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	6	11.01
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	11	10.84
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	18	10.83
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	20	10.68
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	4	10.66
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	17	10.62
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	18	10.6
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	14	10.49
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	7	10.18
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	8	10.15
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	2	9.9
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	1	9.74
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	15	9.68
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	20	8.9
(1,79)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:GLY:N	3	8.75
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	7	8.57
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1	8.4
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	11	7.96
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	5	7.74
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	2	7.62
(1,52)	1:103:A:GLU:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	6	7.58
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	14	7.51
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	20	7.15
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	11	7.06
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	12	6.9
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	10	6.82
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	7	6.7
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	18	6.56
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1	6.48
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	5	6.38
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	12	6.08
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	9	6.03
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	3	5.95
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	18	5.94
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	6	5.71
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	11	5.66
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	20	5.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	13	5.46
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	15	5.42
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	20	5.39
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	14	5.38
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	9	5.37
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	14	5.27
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	4	5.22
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	20	5.15
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	18	5.08
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	13	5.06
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	10	5.02
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	4	5.02
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	16	4.96
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	14	4.96
(1,93)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:LYS:N	16	4.9
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	15	4.9
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	19	4.9
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	18	4.9
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	4	4.89
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	16	4.89
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	2	4.87
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	9	4.83
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	6	4.8
(1,52)	1:103:A:GLU:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	3	4.8
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	17	4.72
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	19	4.72
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	3	4.71
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	9	4.7
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	16	4.69
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	19	4.69
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	8	4.68
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	8	4.66
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	6	4.64
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	3	4.63
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	4	4.6
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	11	4.6
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	16	4.6
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	7	4.57
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	12	4.49
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	8	4.49
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	1	4.42
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	7	4.42
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	13	4.42
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	6	4.38
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	18	4.38
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	14	4.37
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	17	4.37
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	3	4.34
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	4	4.3
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	12	4.29
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	9	4.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	1	4.25
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	13	4.24
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	19	4.22
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	12	4.21
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	9	4.19
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	15	4.18
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	7	4.18
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	12	4.17
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	10	4.17
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	6	4.16
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	15	4.15
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	16	4.13
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	15	4.12
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	13	3.99
(1,101)	1:84:A:ASP:N	1:84:A:ASP:CA	1:84:A:ASP:C	1:85:A:MET:N	9	3.96
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	13	3.94
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	10	3.92
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	5	3.9
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	12	3.82
(1,82)	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	1:49:A:ASP:N	15	3.81
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	9	3.81
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	18	3.79
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	3	3.75
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	20	3.72
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	11	3.68
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	10	3.67
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	9	3.65
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	3	3.61
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	9	3.61
(1,30)	1:59:A:ARG:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	12	3.54
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	2	3.52
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	16	3.48
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	15	3.48
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	15	3.48
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	8	3.48
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	17	3.46
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	12	3.42
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	7	3.4
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	9	3.4
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	12	3.4
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	14	3.39
(1,51)	1:96:A:ARG:C	1:97:A:LEU:N	1:97:A:LEU:CA	1:97:A:LEU:C	11	3.39
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	13	3.33
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	4	3.33
(1,54)	1:105:A:VAL:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	17	3.33
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	11	3.28
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	3	3.26
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	20	3.23
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	8	3.19
(1,77)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ILE:N	19	3.16
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	19	3.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	2	3.13
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	13	3.13
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	1	3.12
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	17	3.11
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	20	3.1
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	2	3.08
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	7	3.06
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	16	3.05
(1,56)	1:107:A:LEU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	6	3.05
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	8	3.03
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	2	3.03
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	14	3.02
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	8	3.01
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	10	3.0
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	7	2.97
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	7	2.97
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	11	2.97
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	9	2.96
(1,93)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:LYS:N	11	2.95
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	19	2.95
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	11	2.94
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	15	2.92
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	4	2.92
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	8	2.91
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	20	2.89
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	11	2.89
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	16	2.84
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	12	2.83
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	4	2.81
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	15	2.79
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	8	2.79
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	18	2.78
(1,86)	1:59:A:ARG:N	1:59:A:ARG:CA	1:59:A:ARG:C	1:60:A:VAL:N	8	2.75
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	10	2.75
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	20	2.75
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	16	2.73
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	19	2.71
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	16	2.7
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	8	2.69
(1,26)	1:55:A:ILE:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	3	2.68
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	16	2.64
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	1	2.62
(1,47)	1:92:A:GLN:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	12	2.62
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	4	2.62
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	17	2.57
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	18	2.56
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	13	2.56
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	4	2.55
(1,30)	1:59:A:ARG:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	7	2.55
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	19	2.54
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	10	2.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	13	2.54
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	15	2.53
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	2	2.53
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	7	2.53
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	20	2.52
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	14	2.52
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	9	2.51
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	20	2.5
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	18	2.49
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	18	2.47
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	13	2.46
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	16	2.45
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	14	2.42
(1,77)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ILE:N	5	2.39
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	3	2.38
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	19	2.36
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	6	2.32
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	10	2.3
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	1	2.27
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	1	2.27
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	8	2.26
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	7	2.24
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	3	2.23
(1,18)	1:31:A:PHE:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	13	2.23
(1,59)	1:110:A:THR:C	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	12	2.22
(1,26)	1:55:A:ILE:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	19	2.21
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	20	2.2
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	3	2.19
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	4	2.18
(1,101)	1:84:A:ASP:N	1:84:A:ASP:CA	1:84:A:ASP:C	1:85:A:MET:N	8	2.16
(1,26)	1:55:A:ILE:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	17	2.16
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	10	2.14
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	17	2.13
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	9	2.13
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	20	2.12
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	19	2.1
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	2	2.06
(1,93)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:LYS:N	20	2.06
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	13	2.06
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	8	2.06
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	17	2.05
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	15	2.05
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	15	2.04
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	18	2.04
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	6	2.04
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	18	2.03
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	7	2.0
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	15	2.0
(1,105)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:ALA:N	19	1.98
(1,8)	1:16:A:VAL:C	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	9	1.98
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	5	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	3	1.95
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	2	1.95
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	8	1.95
(1,86)	1:59:A:ARG:N	1:59:A:ARG:CA	1:59:A:ARG:C	1:60:A:VAL:N	13	1.93
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	7	1.92
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	18	1.91
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1	1.91
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	12	1.9
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	12	1.9
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	4	1.89
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	16	1.87
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	11	1.86
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	14	1.85
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	10	1.82
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	10	1.82
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	5	1.82
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	14	1.81
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	1	1.8
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	12	1.8
(1,23)	1:46:A:PHE:C	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	14	1.78
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	4	1.77
(1,59)	1:110:A:THR:C	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	4	1.76
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	18	1.75
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	20	1.74
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	20	1.74
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	17	1.73
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	5	1.73
(1,57)	1:108:A:LEU:C	1:109:A:VAL:N	1:109:A:VAL:CA	1:109:A:VAL:C	20	1.73
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	17	1.72
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	6	1.71
(1,93)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:LYS:N	8	1.7
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	8	1.67
(1,9)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	6	1.67
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	18	1.66
(1,73)	1:26:A:ASN:N	1:26:A:ASN:CA	1:26:A:ASN:C	1:27:A:LEU:N	15	1.66
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	2	1.65
(1,88)	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	1:62:A:GLU:N	16	1.64
(1,45)	1:90:A:HIS:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	8	1.64
(1,72)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:GLY:N	6	1.63
(1,20)	1:33:A:ILE:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	19	1.63
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	3	1.62
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	16	1.61
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	7	1.59
(1,86)	1:59:A:ARG:N	1:59:A:ARG:CA	1:59:A:ARG:C	1:60:A:VAL:N	7	1.59
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	5	1.59
(1,105)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:ALA:N	5	1.56
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	9	1.56
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	9	1.55
(1,22)	1:35:A:GLY:C	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	5	1.53
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	20	1.53
(1,8)	1:16:A:VAL:C	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	17	1.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	2	1.52
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	14	1.51
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	19	1.48
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	11	1.48
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	1	1.47
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	1	1.46
(1,20)	1:33:A:ILE:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	12	1.46
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	6	1.45
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	7	1.45
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1	1.44
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	8	1.43
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	7	1.42
(1,45)	1:90:A:HIS:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	10	1.42
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	11	1.39
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	7	1.38
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	11	1.38
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	10	1.37
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	13	1.37
(1,58)	1:109:A:VAL:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	6	1.36
(1,45)	1:90:A:HIS:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	17	1.36
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	19	1.36
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	7	1.35
(1,55)	1:106:A:ARG:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	5	1.34
(1,35)	1:75:A:ASP:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	15	1.34
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	2	1.33
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	13	1.33
(1,86)	1:59:A:ARG:N	1:59:A:ARG:CA	1:59:A:ARG:C	1:60:A:VAL:N	15	1.31
(1,9)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	11	1.31
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	7	1.3
(1,17)	1:30:A:GLY:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	3	1.3
(1,117)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ARG:N	8	1.29
(1,24)	1:47:A:SER:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	14	1.28
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	17	1.26
(1,102)	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	1:86:A:THR:N	9	1.25
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	3	1.25
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	20	1.23
(1,83)	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	1:56:A:TYR:N	3	1.23
(1,15)	1:26:A:ASN:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	10	1.22
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	19	1.22
(1,104)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:GLN:N	11	1.21
(1,82)	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	1:49:A:ASP:N	8	1.21
(1,82)	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	1:49:A:ASP:N	9	1.21
(1,115)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:VAL:N	16	1.2
(1,52)	1:103:A:GLU:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	10	1.2
(1,60)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:ALA:N	11	1.19
(1,56)	1:107:A:LEU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	18	1.19
(1,47)	1:92:A:GLN:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	2	1.19
(1,94)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:ILE:N	16	1.18
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	9	1.16
(1,101)	1:84:A:ASP:N	1:84:A:ASP:CA	1:84:A:ASP:C	1:85:A:MET:N	20	1.12
(1,35)	1:75:A:ASP:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	12	1.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:84:A:ASP:N	1:84:A:ASP:CA	1:84:A:ASP:C	1:85:A:MET:N	12	1.1
(1,61)	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1:12:A:VAL:N	11	1.1
(1,36)	1:76:A:LYS:C	1:77:A:ILE:N	1:77:A:ILE:CA	1:77:A:ILE:C	6	1.1
(1,34)	1:74:A:GLY:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	5	1.1
(1,6)	1:14:A:GLN:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	6	1.1
(1,19)	1:32:A:SER:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	6	1.09
(1,8)	1:16:A:VAL:C	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	4	1.08
(1,109)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:LEU:N	5	1.07
(1,16)	1:27:A:LEU:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	17	1.07
(1,45)	1:90:A:HIS:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	13	1.05
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	20	1.05
(1,26)	1:55:A:ILE:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	15	1.05
(1,11)	1:20:A:LYS:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	17	1.05
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	13	1.04
(1,64)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	3	1.04
(1,50)	1:95:A:LYS:C	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	17	1.03
(1,20)	1:33:A:ILE:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	5	1.02
(1,81)	1:47:A:SER:N	1:47:A:SER:CA	1:47:A:SER:C	1:48:A:GLU:N	5	1.01
(1,80)	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	1:36:A:GLY:N	2	1.01
(1,43)	1:84:A:ASP:C	1:85:A:MET:N	1:85:A:MET:CA	1:85:A:MET:C	14	1.01
(1,8)	1:16:A:VAL:C	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	7	1.01
(1,4)	1:12:A:VAL:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	6	1.01