



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:03 AM UTC

PDB ID : 2IZ3 / pdb_00002iz3
BMRB ID : 15037
Title : Solution structure of human beta-microseminoprotein
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Deposited on : 2006-07-24

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

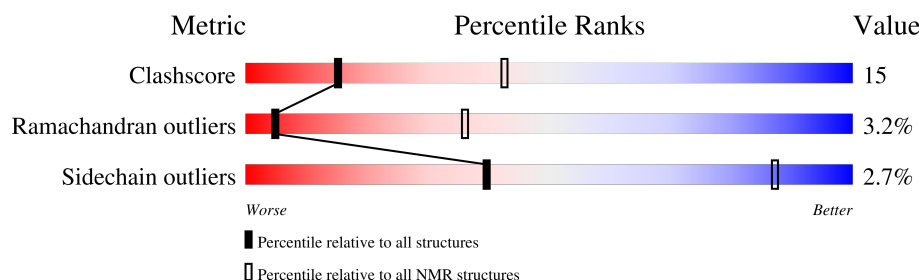
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 38%.

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	97	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:7, A:18-A:94 (83)	0.97	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 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1460 atoms, of which 713 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BETA-MICROSEMINOPROTEIN.

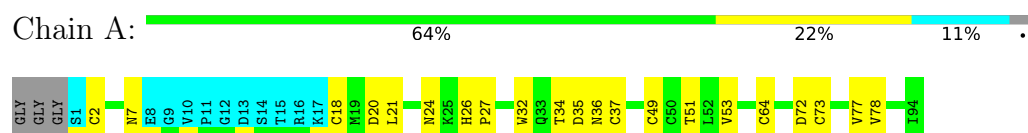
Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1460	463	713	122	151	11	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: BETA-MICROSEMINOPROTEIN

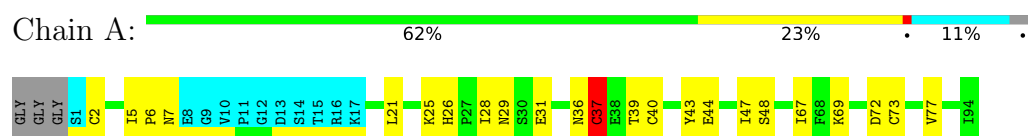


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

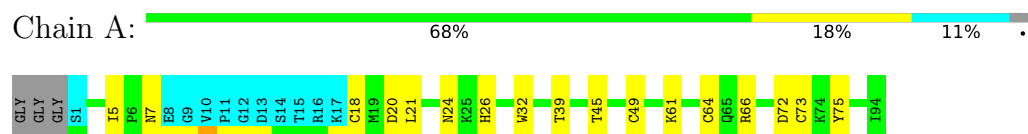
4.2.1 Score per residue for model 1

- Molecule 1: BETA-MICROSEMINOPROTEIN



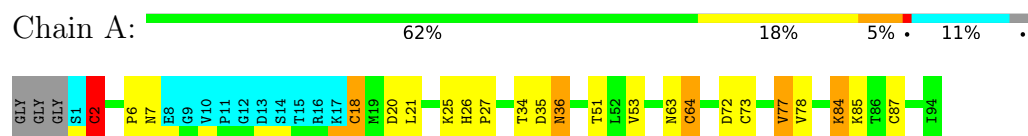
4.2.2 Score per residue for model 2

- Molecule 1: BETA-MICROSEMINOPROTEIN



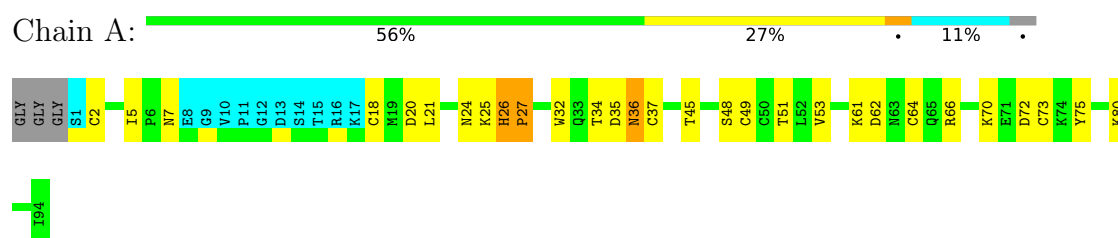
4.2.3 Score per residue for model 3

- Molecule 1: BETA-MICROSEMINOPROTEIN



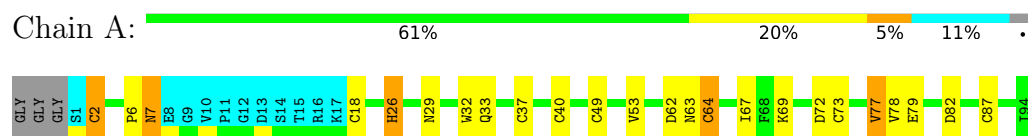
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: BETA-MICROSEMINOPROTEIN



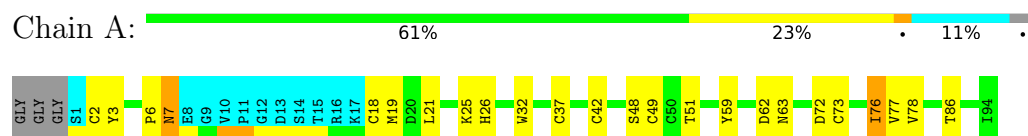
4.2.5 Score per residue for model 5

- Molecule 1: BETA-MICROSEMINOPROTEIN



4.2.6 Score per residue for model 6

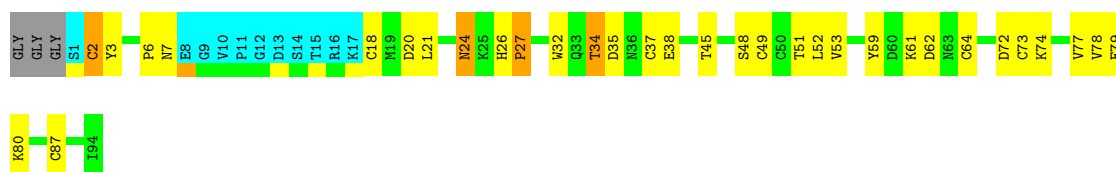
- Molecule 1: BETA-MICROSEMINOPROTEIN



4.2.7 Score per residue for model 7

- Molecule 1: BETA-MICROSEMINOPROTEIN

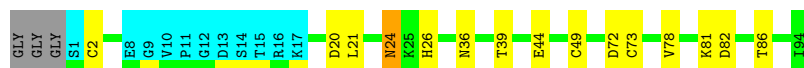




4.2.8 Score per residue for model 8

- Molecule 1: BETA-MICROSEMINOPROTEIN

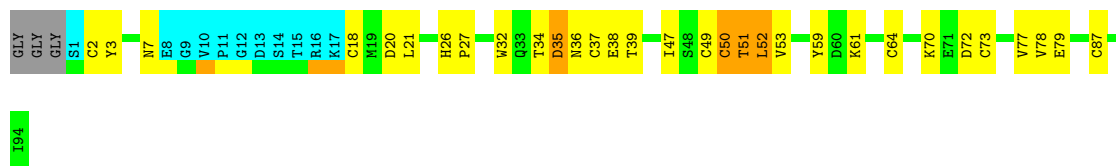
Chain A: 70% 14% 11%



4.2.9 Score per residue for model 9

- Molecule 1: BETA-MICROSEMINOPROTEIN

Chain A: 54% 28% 11%



4.2.10 Score per residue for model 10

- Molecule 1: BETA-MICROSEMINOPROTEIN

Chain A: 54% 30% 11%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ANNEALING*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *LOW ENERGY AND NO VIOLATIONS* > 0.5 Å.

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

Software name	Classification	Version
Xplor-NIH	refinement	
Xplor-NIH	structure solution	

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	467
Number of shifts mapped to atoms	467
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	669	638	637	19±6
All	All	6690	6380	6370	194

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:HIS:CE1	1:A:32:TRP:CZ2	0.66	2.84	4	2
1:A:53:VAL:HG12	1:A:73:CYS:C	0.66	2.15	9	2
1:A:26:HIS:CE1	1:A:32:TRP:CH2	0.65	2.84	5	4
1:A:26:HIS:CG	1:A:32:TRP:CE3	0.64	2.85	4	3
1:A:63:ASN:O	1:A:64:CYS:SG	0.63	2.56	5	2
1:A:66:ARG:NH2	1:A:75:TYR:CZ	0.62	2.67	4	1
1:A:51:THR:O	1:A:53:VAL:N	0.62	2.32	4	3
1:A:26:HIS:CD2	1:A:32:TRP:CD2	0.61	2.87	2	4
1:A:66:ARG:NH2	1:A:75:TYR:CE2	0.60	2.69	4	1
1:A:32:TRP:CH2	1:A:42:CYS:SG	0.59	2.95	6	1
1:A:79:GLU:N	1:A:87:CYS:SG	0.59	2.75	7	2
1:A:26:HIS:ND1	1:A:32:TRP:CH2	0.58	2.71	4	1
1:A:26:HIS:ND1	1:A:32:TRP:CZ3	0.58	2.72	7	2
1:A:24:ASN:ND2	1:A:26:HIS:CE1	0.56	2.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLU:CD	1:A:44:GLU:H	0.55	2.10	8	1
1:A:39:THR:HG22	1:A:40:CYS:N	0.55	2.17	1	1
1:A:48:SER:O	1:A:49:CYS:SG	0.54	2.65	10	4
1:A:51:THR:C	1:A:53:VAL:H	0.54	2.11	10	3
1:A:21:LEU:CD2	1:A:21:LEU:N	0.54	2.71	8	2
1:A:18:CYS:O	1:A:26:HIS:CE1	0.54	2.60	4	2
1:A:78:VAL:CA	1:A:87:CYS:SG	0.53	2.97	5	2
1:A:20:ASP:OD1	1:A:24:ASN:ND2	0.53	2.41	8	1
1:A:18:CYS:SG	1:A:18:CYS:O	0.53	2.66	2	4
1:A:26:HIS:CG	1:A:32:TRP:CZ3	0.53	2.96	4	2
1:A:59:TYR:CE2	1:A:77:VAL:HG11	0.53	2.38	7	4
1:A:67:ILE:HG21	1:A:69:LYS:NZ	0.53	2.18	5	2
1:A:34:THR:O	1:A:36:ASN:N	0.52	2.42	4	1
1:A:31:GLU:N	1:A:31:GLU:OE1	0.52	2.43	1	1
1:A:20:ASP:OD1	1:A:21:LEU:N	0.52	2.42	2	4
1:A:39:THR:O	1:A:49:CYS:SG	0.52	2.67	9	3
1:A:24:ASN:O	1:A:24:ASN:ND2	0.52	2.42	7	1
1:A:25:LYS:O	1:A:26:HIS:ND1	0.52	2.42	3	2
1:A:77:VAL:C	1:A:87:CYS:SG	0.52	2.92	3	2
1:A:51:THR:C	1:A:53:VAL:N	0.52	2.68	7	2
1:A:24:ASN:HD22	1:A:24:ASN:C	0.52	2.12	4	2
1:A:18:CYS:HB3	1:A:47:ILE:HD11	0.52	1.82	9	1
1:A:26:HIS:NE2	1:A:32:TRP:CE2	0.52	2.77	2	2
1:A:21:LEU:N	1:A:21:LEU:HD22	0.52	2.19	8	2
1:A:62:ASP:O	1:A:80:LYS:NZ	0.52	2.42	4	3
1:A:3:TYR:CD1	1:A:3:TYR:N	0.52	2.76	10	2
1:A:2:CYS:SG	1:A:49:CYS:C	0.51	2.93	4	2
1:A:2:CYS:SG	1:A:49:CYS:O	0.51	2.68	6	1
1:A:51:THR:OG1	1:A:52:LEU:N	0.51	2.39	9	1
1:A:40:CYS:SG	1:A:48:SER:O	0.51	2.69	1	1
1:A:39:THR:C	1:A:49:CYS:SG	0.51	2.94	2	3
1:A:24:ASN:C	1:A:24:ASN:ND2	0.50	2.69	4	2
1:A:40:CYS:SG	1:A:48:SER:C	0.50	2.95	1	1
1:A:18:CYS:O	1:A:18:CYS:SG	0.50	2.70	4	1
1:A:34:THR:O	1:A:35:ASP:O	0.49	2.30	9	1
1:A:66:ARG:NH1	1:A:75:TYR:CE1	0.49	2.81	2	1
1:A:24:ASN:ND2	1:A:26:HIS:NE2	0.49	2.60	8	1
1:A:21:LEU:N	1:A:21:LEU:HD12	0.49	2.23	9	4
1:A:78:VAL:HG12	1:A:86:THR:HA	0.49	1.85	10	3
1:A:28:ILE:HG22	1:A:29:ASN:N	0.49	2.22	1	1
1:A:37:CYS:O	1:A:38:GLU:CD	0.48	2.55	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:C	1:A:87:CYS:SG	0.48	2.96	5	4
1:A:35:ASP:O	1:A:36:ASN:CB	0.48	2.60	3	2
1:A:37:CYS:O	1:A:51:THR:O	0.48	2.31	4	1
1:A:7:ASN:OD1	1:A:46:GLU:N	0.48	2.45	10	1
1:A:82:ASP:N	1:A:82:ASP:OD1	0.48	2.46	5	1
1:A:26:HIS:CD2	1:A:32:TRP:CE3	0.48	3.02	2	1
1:A:33:GLN:N	1:A:33:GLN:CD	0.47	2.73	5	1
1:A:62:ASP:OD1	1:A:63:ASN:N	0.47	2.47	6	1
1:A:26:HIS:CB	1:A:32:TRP:CE3	0.47	2.97	4	1
1:A:32:TRP:CZ3	1:A:42:CYS:SG	0.47	3.08	6	1
1:A:20:ASP:CG	1:A:24:ASN:HD21	0.47	2.18	8	1
1:A:7:ASN:OD1	1:A:7:ASN:O	0.47	2.33	5	2
1:A:25:LYS:C	1:A:26:HIS:CG	0.47	2.93	1	3
1:A:37:CYS:SG	1:A:70:LYS:O	0.47	2.73	4	1
1:A:77:VAL:O	1:A:87:CYS:N	0.46	2.48	10	1
1:A:34:THR:C	1:A:36:ASN:H	0.46	2.18	3	1
1:A:36:ASN:OD1	1:A:37:CYS:N	0.46	2.49	10	1
1:A:72:ASP:O	1:A:73:CYS:C	0.46	2.59	10	10
1:A:61:LYS:O	1:A:64:CYS:O	0.46	2.33	9	5
1:A:6:PRO:O	1:A:7:ASN:C	0.46	2.58	6	2
1:A:36:ASN:O	1:A:37:CYS:SG	0.45	2.74	1	1
1:A:50:CYS:O	1:A:51:THR:O	0.45	2.34	9	1
1:A:21:LEU:N	1:A:21:LEU:CD1	0.45	2.80	9	2
1:A:39:THR:CG2	1:A:40:CYS:N	0.45	2.80	1	1
1:A:43:TYR:O	1:A:44:GLU:C	0.45	2.59	1	1
1:A:34:THR:O	1:A:38:GLU:O	0.43	2.36	9	2
1:A:3:TYR:CD1	1:A:3:TYR:O	0.43	2.71	7	1
1:A:79:GLU:OE1	1:A:82:ASP:OD1	0.43	2.37	5	1
1:A:29:ASN:OD1	1:A:29:ASN:O	0.43	2.37	5	1
1:A:84:LYS:CG	1:A:85:LYS:N	0.43	2.82	3	1
1:A:45:THR:O	1:A:45:THR:OG1	0.43	2.36	7	2
1:A:72:ASP:O	1:A:74:LYS:NZ	0.43	2.51	7	1
1:A:44:GLU:CD	1:A:44:GLU:N	0.43	2.76	8	1
1:A:26:HIS:O	1:A:27:PRO:O	0.43	2.36	4	2
1:A:7:ASN:O	1:A:7:ASN:OD1	0.43	2.35	1	1
1:A:3:TYR:CD1	1:A:3:TYR:C	0.43	2.97	6	2
1:A:18:CYS:CB	1:A:47:ILE:HD11	0.43	2.44	9	1
1:A:35:ASP:C	1:A:36:ASN:CG	0.42	2.87	10	1
1:A:24:ASN:HD22	1:A:25:LYS:N	0.42	2.13	4	1
1:A:36:ASN:O	1:A:38:GLU:OE2	0.42	2.37	9	1
1:A:51:THR:OG1	1:A:53:VAL:HG22	0.42	2.14	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ILE:HD13	1:A:76:ILE:N	0.42	2.29	6	1
1:A:26:HIS:CE1	1:A:32:TRP:CZ3	0.42	3.08	7	1
1:A:60:ASP:OD1	1:A:60:ASP:N	0.41	2.53	10	1
1:A:60:ASP:OD1	1:A:87:CYS:SG	0.41	2.78	10	1
1:A:40:CYS:SG	1:A:47:ILE:CG2	0.41	3.08	1	1
1:A:24:ASN:C	1:A:24:ASN:HD22	0.41	2.23	2	1
1:A:34:THR:OG1	1:A:36:ASN:OD1	0.41	2.37	10	1
1:A:44:GLU:N	1:A:44:GLU:OE1	0.41	2.42	8	1
1:A:35:ASP:OD2	1:A:38:GLU:OE1	0.41	2.39	7	1
1:A:75:TYR:O	1:A:92:TRP:CH2	0.41	2.74	10	1
1:A:62:ASP:OD1	1:A:62:ASP:O	0.41	2.38	5	1
1:A:59:TYR:CZ	1:A:77:VAL:HG11	0.41	2.51	7	1
1:A:20:ASP:OD1	1:A:20:ASP:C	0.41	2.63	9	1
1:A:7:ASN:OD1	1:A:7:ASN:C	0.41	2.62	2	1
1:A:81:LYS:O	1:A:82:ASP:OD1	0.41	2.39	8	1
1:A:36:ASN:OD1	1:A:70:LYS:NZ	0.41	2.43	9	1
1:A:7:ASN:OD1	1:A:45:THR:C	0.41	2.64	10	1
1:A:53:VAL:CG1	1:A:54:SER:N	0.40	2.85	10	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	82/97 (85%)	74±2 (90±3%)	5±1 (6±2%)	3±2 (3±2%)	5	36
All	All	820/970 (85%)	742 (90%)	52 (6%)	26 (3%)	5	36

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	CYS	5
1	A	7	ASN	4
1	A	27	PRO	4
1	A	36	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	64	CYS	2
1	A	35	ASP	2
1	A	52	LEU	2
1	A	37	CYS	1
1	A	18	CYS	1
1	A	51	THR	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/90 (90%)	79±1 (97±2%)	2±1 (3±2%)	40	87
All	All	810/900 (90%)	788 (97%)	22 (3%)	40	87

All 13 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	37	CYS	4
1	A	77	VAL	3
1	A	2	CYS	2
1	A	26	HIS	2
1	A	24	ASN	2
1	A	50	CYS	2
1	A	45	THR	1
1	A	84	LYS	1
1	A	40	CYS	1
1	A	49	CYS	1
1	A	76	ILE	1
1	A	34	THR	1
1	A	52	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	467
Number of shifts mapped to atoms	467
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 38%, i.e. 419 atoms were assigned a chemical shift out of a possible 1100. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	151/409 (37%)	151/164 (92%)	0/166 (0%)	0/79 (0%)
Sidechain	256/603 (42%)	256/386 (66%)	0/197 (0%)	0/20 (0%)
Aromatic	12/88 (14%)	12/42 (29%)	0/42 (0%)	0/4 (0%)
Overall	419/1100 (38%)	419/592 (71%)	0/405 (0%)	0/103 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 467 atoms were assigned a chemical shift out of a possible 1228. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	172/464 (37%)	172/187 (92%)	0/188 (0%)	0/89 (0%)
Sidechain	283/676 (42%)	283/432 (66%)	0/220 (0%)	0/24 (0%)
Aromatic	12/88 (14%)	12/42 (29%)	0/42 (0%)	0/4 (0%)
Overall	467/1228 (38%)	467/661 (71%)	0/450 (0%)	0/117 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

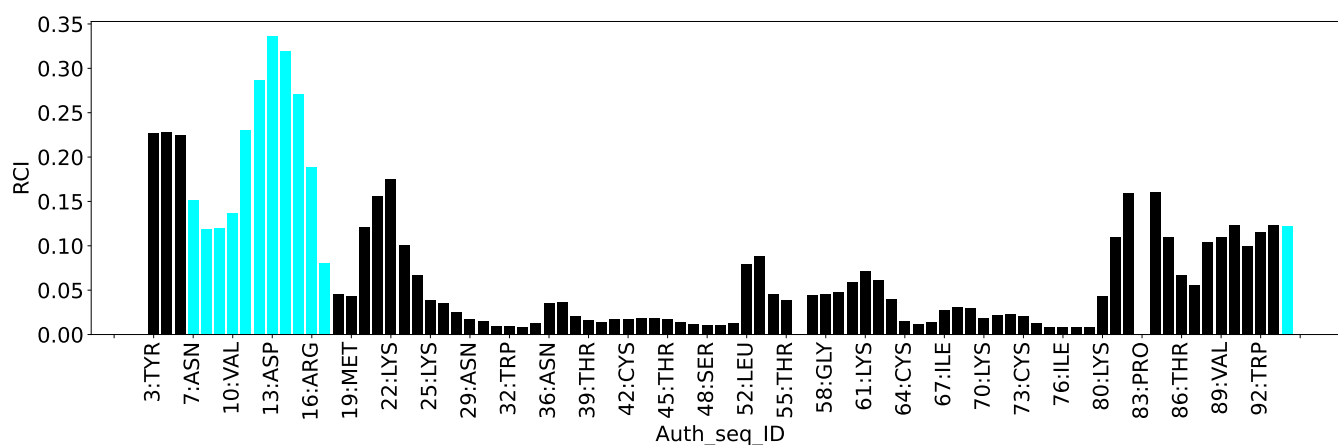
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	40	CYS	HB2	0.50	0.81 – 5.11	-5.7

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	1562
Intra-residue ($ i-j =0$)	351
Sequential ($ i-j =1$)	398
Medium range ($ i-j >1$ and $ i-j <5$)	211
Long range ($ i-j \geq 5$)	602
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.1
Number of long range restraints per residue ¹	6.2

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)	19.8	0.2
0.2-0.5 (Medium)	28.5	0.5
>0.5 (Large)	34.5	1.57

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

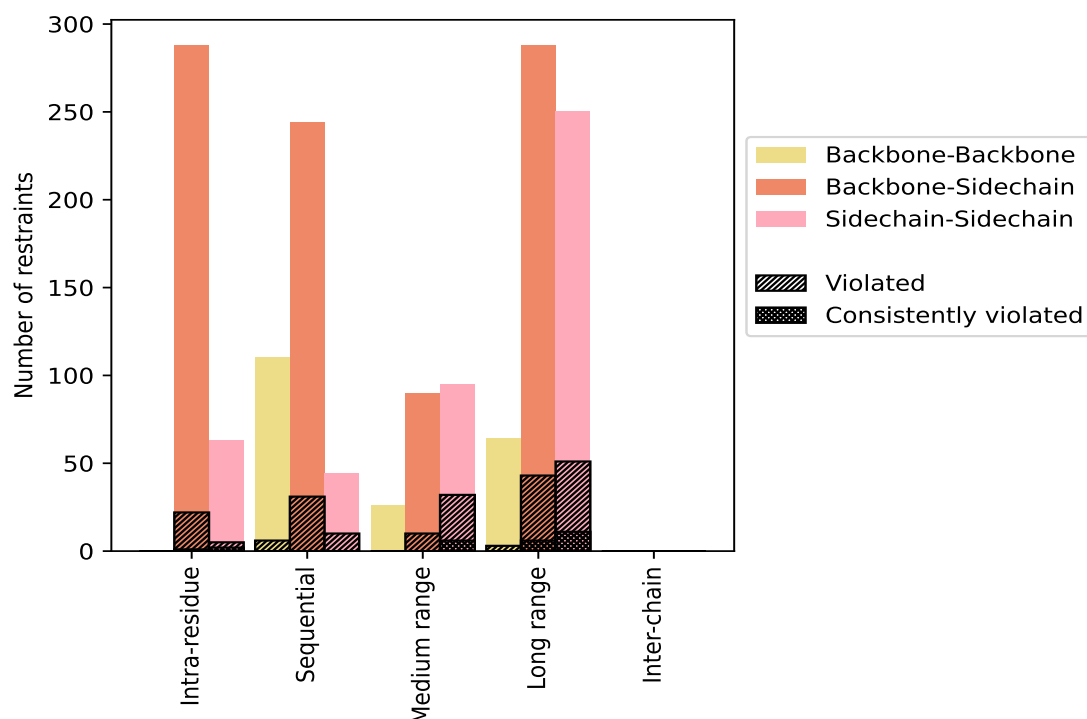
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	351	22.5	27	7.7	1.7	3	0.9	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	288	18.4	22	7.6	1.4	1	0.3	0.1
Sidechain-Sidechain	63	4.0	5	7.9	0.3	2	3.2	0.1
Sequential ($i-j =1$)	398	25.5	47	11.8	3.0	0	0.0	0.0
Backbone-Backbone	110	7.0	6	5.5	0.4	0	0.0	0.0
Backbone-Sidechain	244	15.6	31	12.7	2.0	0	0.0	0.0
Sidechain-Sidechain	44	2.8	10	22.7	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	211	13.5	42	19.9	2.7	6	2.8	0.4
Backbone-Backbone	26	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	90	5.8	10	11.1	0.6	0	0.0	0.0
Sidechain-Sidechain	95	6.1	32	33.7	2.0	6	6.3	0.4
Long range ($i-j \geq 5$)	602	38.5	97	16.1	6.2	17	2.8	1.1
Backbone-Backbone	64	4.1	3	4.7	0.2	0	0.0	0.0
Backbone-Sidechain	288	18.4	43	14.9	2.8	6	2.1	0.4
Sidechain-Sidechain	250	16.0	51	20.4	3.3	11	4.4	0.7
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1562	100.0	213	13.6	13.6	26	1.7	1.7
Backbone-Backbone	200	12.8	9	4.5	0.6	0	0.0	0.0
Backbone-Sidechain	910	58.3	106	11.6	6.8	7	0.8	0.4
Sidechain-Sidechain	452	28.9	98	21.7	6.3	19	4.2	1.2

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

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



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

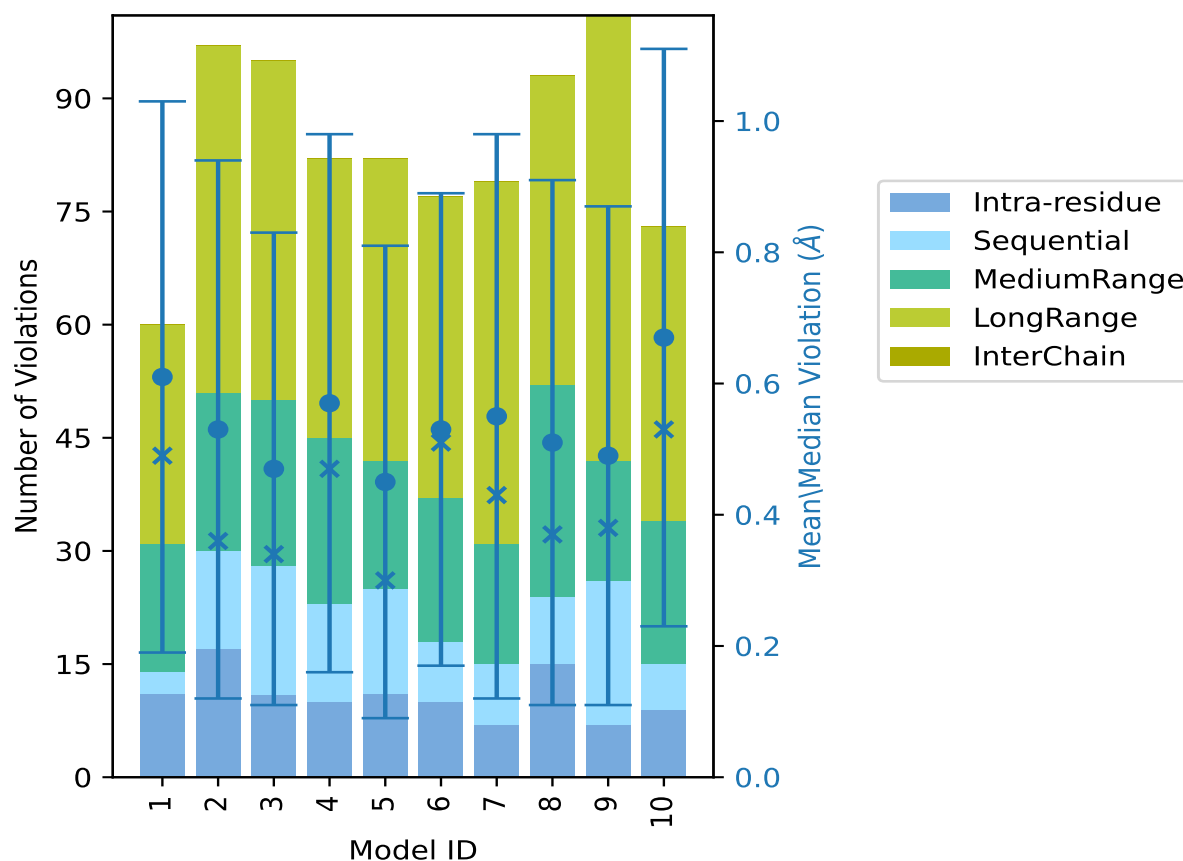
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	11	3	17	29	0	60	0.61	1.53	0.42	0.49
2	17	13	21	46	0	97	0.53	1.44	0.41	0.36
3	11	17	22	45	0	95	0.47	1.39	0.36	0.34
4	10	13	22	37	0	82	0.57	1.41	0.41	0.47
5	11	14	17	40	0	82	0.45	1.42	0.36	0.3
6	10	8	19	40	0	77	0.53	1.49	0.36	0.51
7	7	8	16	48	0	79	0.55	1.57	0.43	0.43
8	15	9	28	41	0	93	0.51	1.42	0.4	0.37
9	7	19	16	59	0	101	0.49	1.52	0.38	0.38
10	9	6	19	39	0	73	0.67	1.54	0.44	0.53

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1349(IR:324, SQ:351, MR:169, LR:505, 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	%
7	19	9	19	0	54	1	10.0
4	12	6	21	0	43	2	20.0
3	8	1	18	0	30	3	30.0

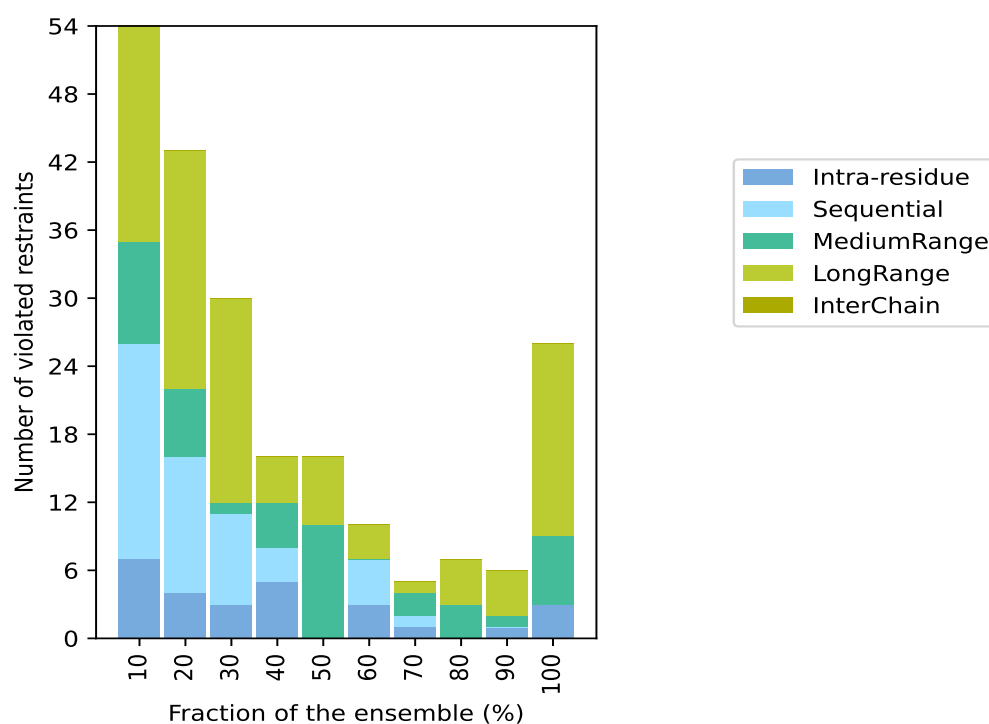
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	3	4	4	0	16	4	40.0
0	0	10	6	0	16	5	50.0
3	4	0	3	0	10	6	60.0
1	1	2	1	0	5	7	70.0
0	0	3	4	0	7	8	80.0
1	0	1	4	0	6	9	90.0
3	0	6	17	0	26	10	100.0

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 ⓘ

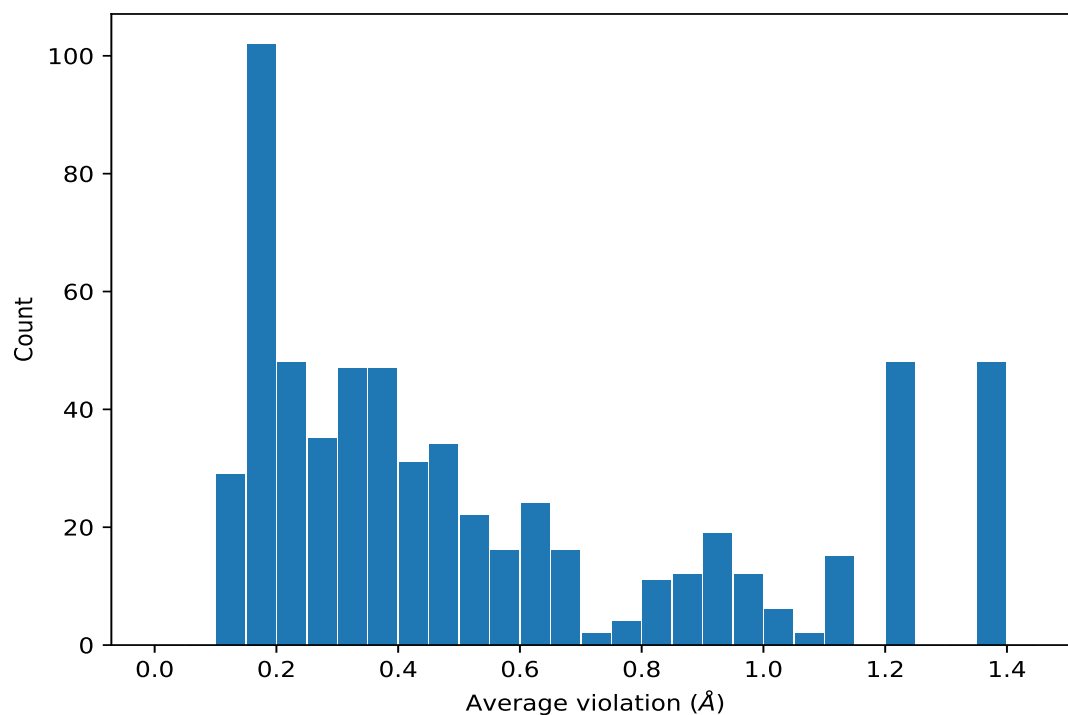


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance 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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.39	0.14	1.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.39	0.14	1.4
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.39	0.14	1.4
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.24	0.34	1.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.24	0.34	1.33
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.24	0.34	1.33
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	10	0.95	0.44	1.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	10	0.95	0.44	1.13
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	10	0.7	0.11	0.76
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	10	0.61	0.08	0.62
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	10	0.61	0.08	0.62
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	10	0.61	0.08	0.62
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	10	0.61	0.08	0.62
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	10	0.61	0.08	0.62
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	10	0.61	0.08	0.62
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	10	0.61	0.08	0.62
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	10	0.54	0.24	0.53
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	10	0.54	0.24	0.53
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	10	0.54	0.24	0.53
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	10	0.54	0.24	0.53
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	10	0.53	0.12	0.54
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	10	0.46	0.12	0.5
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	10	0.46	0.12	0.5
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	10	0.46	0.12	0.5
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	10	0.46	0.12	0.5
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	10	0.46	0.12	0.5
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	10	0.46	0.12	0.5
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	10	0.4	0.15	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	10	0.4	0.15	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	10	0.4	0.15	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	10	0.4	0.15	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	10	0.4	0.15	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	10	0.4	0.15	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	10	0.4	0.15	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	10	0.4	0.15	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	10	0.4	0.15	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	10	0.4	0.15	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	10	0.4	0.15	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	10	0.4	0.15	0.48
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	10	0.38	0.01	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	10	0.38	0.01	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	10	0.38	0.01	0.38
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	10	0.37	0.11	0.33
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	10	0.37	0.11	0.33
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	10	0.37	0.11	0.33
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	10	0.37	0.11	0.33
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	10	0.34	0.16	0.4
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	10	0.34	0.16	0.4
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	10	0.34	0.16	0.4
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	10	0.34	0.16	0.4
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	10	0.34	0.16	0.4
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	10	0.34	0.16	0.4
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	10	0.34	0.16	0.4
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	10	0.34	0.16	0.4
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	10	0.18	0.0	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	10	0.18	0.0	0.18
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	9	1.07	0.27	1.15
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	9	1.07	0.27	1.15
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	9	0.92	0.33	0.81
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	9	0.92	0.33	0.81
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	9	0.92	0.33	0.81
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	9	0.58	0.04	0.6
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	9	0.58	0.04	0.6
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	9	0.48	0.08	0.49
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	9	0.48	0.08	0.49
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	9	0.27	0.03	0.28
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	9	0.27	0.03	0.28
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	9	0.27	0.03	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	9	0.27	0.03	0.28
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	8	0.87	0.28	0.75
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	8	0.87	0.28	0.75
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	8	0.87	0.28	0.75
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	8	0.87	0.28	0.75
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	8	0.87	0.28	0.75
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	8	0.87	0.28	0.75
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	8	0.87	0.28	0.75
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	8	0.33	0.14	0.26
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	8	0.33	0.14	0.26
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	8	0.33	0.14	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	8	0.33	0.14	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	8	0.33	0.14	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	8	0.33	0.14	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	8	0.33	0.14	0.26
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	8	0.23	0.02	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	8	0.23	0.02	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	8	0.23	0.02	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	8	0.23	0.02	0.23
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	8	0.2	0.05	0.2
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	8	0.2	0.05	0.2
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	7	0.68	0.1	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	7	0.68	0.1	0.7
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	7	0.68	0.1	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	7	0.68	0.1	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	7	0.68	0.1	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	7	0.68	0.1	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	7	0.68	0.1	0.7
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	7	0.6	0.04	0.59
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	7	0.6	0.04	0.59
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	7	0.6	0.04	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	7	0.59	0.06	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	7	0.59	0.06	0.59
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	7	0.25	0.08	0.26
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	6	0.93	0.23	0.99
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	6	0.93	0.23	0.99
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	6	0.93	0.23	0.99
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	6	0.93	0.23	0.99
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	6	0.93	0.23	0.99
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	6	0.93	0.23	0.99
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	6	0.77	0.2	0.71
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	6	0.77	0.2	0.71
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	6	0.77	0.2	0.71
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	6	0.77	0.2	0.71
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	6	0.6	0.06	0.6
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	6	0.6	0.06	0.6
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	6	0.6	0.06	0.6
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	6	0.6	0.06	0.6
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	6	0.6	0.06	0.6
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	6	0.6	0.06	0.6
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	6	0.57	0.24	0.5
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	6	0.57	0.24	0.5
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	6	0.57	0.24	0.5
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	6	0.57	0.24	0.5
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	6	0.57	0.24	0.5
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	6	0.57	0.24	0.5
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	6	0.33	0.14	0.31
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	6	0.33	0.14	0.31
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	6	0.33	0.14	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	6	0.33	0.14	0.31
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	6	0.27	0.09	0.26
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	6	0.27	0.09	0.26
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	6	0.27	0.09	0.26
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	6	0.27	0.09	0.26
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	6	0.27	0.09	0.26
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	6	0.27	0.09	0.26
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	6	0.27	0.09	0.26
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	6	0.16	0.03	0.16
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	6	0.16	0.03	0.16
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	6	0.16	0.03	0.16
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	6	0.16	0.03	0.16
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	6	0.16	0.03	0.16
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	6	0.16	0.03	0.16
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	5	1.12	0.26	1.1
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	5	1.12	0.26	1.1
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	5	1.12	0.26	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	5	1.12	0.26	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	5	1.12	0.26	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	5	1.12	0.26	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	5	1.12	0.26	1.1
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	5	1.04	0.23	1.1
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	5	1.01	0.1	1.05
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	5	0.93	0.01	0.94
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	5	0.93	0.01	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	5	0.93	0.01	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	5	0.93	0.01	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	5	0.93	0.01	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	5	0.93	0.01	0.94
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	5	0.66	0.25	0.54
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	5	0.66	0.25	0.54
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	5	0.66	0.25	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	5	0.66	0.25	0.54
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	5	0.55	0.19	0.6
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	5	0.55	0.19	0.6
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	5	0.55	0.19	0.6
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	5	0.53	0.16	0.54
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	5	0.53	0.16	0.54
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	5	0.53	0.16	0.54
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	5	0.53	0.16	0.54
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	5	0.47	0.19	0.45
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	5	0.47	0.19	0.45
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	5	0.47	0.19	0.45
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	5	0.47	0.19	0.45
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	5	0.47	0.19	0.45
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	5	0.47	0.19	0.45
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	5	0.31	0.05	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	5	0.31	0.05	0.27
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	5	0.16	0.03	0.15
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	5	0.16	0.03	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	5	0.16	0.03	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	5	0.16	0.03	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	5	0.16	0.03	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	5	0.16	0.03	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	5	0.16	0.03	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	5	0.16	0.03	0.15
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	5	0.15	0.01	0.15
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	5	0.15	0.01	0.15
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	5	0.15	0.01	0.15
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	5	0.15	0.01	0.15
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE2	4	1.0	0.07	1.04
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE3	4	1.0	0.07	1.04
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE2	4	1.0	0.07	1.04
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE3	4	1.0	0.07	1.04
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD11	4	0.82	0.06	0.84
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD12	4	0.82	0.06	0.84
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD13	4	0.82	0.06	0.84
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD11	4	0.55	0.26	0.62
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD12	4	0.55	0.26	0.62
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD13	4	0.55	0.26	0.62
(1,135)	1:7:A:ASN:HA	1:47:A:ILE:HG13	4	0.5	0.16	0.52
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	4	0.5	0.19	0.42
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	4	0.5	0.19	0.42
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	4	0.5	0.19	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	4	0.5	0.19	0.42
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	4	0.5	0.19	0.42
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	4	0.5	0.19	0.42
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE1	4	0.4	0.12	0.41
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE2	4	0.4	0.12	0.41
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE1	4	0.4	0.12	0.41
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE2	4	0.4	0.12	0.41
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE1	4	0.4	0.2	0.32
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE2	4	0.4	0.2	0.32
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD2	4	0.39	0.05	0.39
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD3	4	0.39	0.05	0.39
(1,203)	1:12:A:GLY:H	1:13:A:ASP:H	4	0.38	0.21	0.36
(1,1009)	1:60:A:ASP:HB2	1:64:A:CYS:H	4	0.21	0.02	0.22
(1,1009)	1:60:A:ASP:HB3	1:64:A:CYS:H	4	0.21	0.02	0.22
(1,185)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,185)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,185)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,185)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,185)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,185)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,186)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	4	0.19	0.07	0.16
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG2	4	0.19	0.01	0.18
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG3	4	0.19	0.01	0.18
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG2	4	0.15	0.03	0.14
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG3	4	0.15	0.03	0.14
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG2	4	0.11	0.01	0.11
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG3	4	0.11	0.01	0.11
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG2	4	0.11	0.01	0.11
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG3	4	0.11	0.01	0.11
(1,762)	1:51:A:THR:HG21	1:53:A:VAL:HB	3	1.1	0.18	1.19
(1,762)	1:51:A:THR:HG22	1:53:A:VAL:HB	3	1.1	0.18	1.19
(1,762)	1:51:A:THR:HG23	1:53:A:VAL:HB	3	1.1	0.18	1.19
(1,559)	1:36:A:ASN:HB2	1:37:A:CYS:H	3	0.81	0.42	1.09
(1,559)	1:36:A:ASN:HB3	1:37:A:CYS:H	3	0.81	0.42	1.09
(1,560)	1:36:A:ASN:HB2	1:37:A:CYS:H	3	0.81	0.42	1.09
(1,560)	1:36:A:ASN:HB3	1:37:A:CYS:H	3	0.81	0.42	1.09
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD11	3	0.63	0.54	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD12	3	0.63	0.54	0.29
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD13	3	0.63	0.54	0.29
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE2	3	0.46	0.13	0.54
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE3	3	0.46	0.13	0.54
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE2	3	0.46	0.13	0.54
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE3	3	0.46	0.13	0.54
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB2	3	0.41	0.13	0.42
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB3	3	0.41	0.13	0.42
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB2	3	0.41	0.13	0.42
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB3	3	0.41	0.13	0.42
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB2	3	0.41	0.13	0.42
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB3	3	0.41	0.13	0.42
(1,256)	1:19:A:MET:HA	1:26:A:HIS:HD2	3	0.4	0.12	0.37
(1,265)	1:19:A:MET:HE1	1:25:A:LYS:HA	3	0.38	0.16	0.36
(1,265)	1:19:A:MET:HE2	1:25:A:LYS:HA	3	0.38	0.16	0.36
(1,265)	1:19:A:MET:HE3	1:25:A:LYS:HA	3	0.38	0.16	0.36
(1,1093)	1:65:A:GLN:HE21	1:80:A:LYS:HA	3	0.36	0.12	0.41
(1,1093)	1:65:A:GLN:HE22	1:80:A:LYS:HA	3	0.36	0.12	0.41
(1,1094)	1:65:A:GLN:HE21	1:80:A:LYS:HA	3	0.36	0.12	0.41
(1,1094)	1:65:A:GLN:HE22	1:80:A:LYS:HA	3	0.36	0.12	0.41
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG21	3	0.36	0.21	0.34
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG22	3	0.36	0.21	0.34
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG23	3	0.36	0.21	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG21	3	0.36	0.21	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG22	3	0.36	0.21	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG23	3	0.36	0.21	0.34
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	3	0.26	0.16	0.21
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	3	0.26	0.16	0.21
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	3	0.26	0.16	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	3	0.26	0.16	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	3	0.26	0.16	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	3	0.26	0.16	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	3	0.26	0.16	0.21
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB2	3	0.25	0.07	0.26
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB3	3	0.25	0.07	0.26
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB2	3	0.25	0.07	0.26
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB3	3	0.25	0.07	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,153)	1:7:A:ASN:H	1:47:A:ILE:H	3	0.25	0.06	0.27
(1,287)	1:20:A:ASP:HB2	1:21:A:LEU:H	3	0.22	0.1	0.16
(1,287)	1:20:A:ASP:HB3	1:21:A:LEU:H	3	0.22	0.1	0.16
(1,288)	1:20:A:ASP:HB2	1:21:A:LEU:H	3	0.22	0.1	0.16
(1,288)	1:20:A:ASP:HB3	1:21:A:LEU:H	3	0.22	0.1	0.16
(1,262)	1:19:A:MET:HE1	1:24:A:ASN:HA	3	0.21	0.07	0.18
(1,262)	1:19:A:MET:HE2	1:24:A:ASN:HA	3	0.21	0.07	0.18
(1,262)	1:19:A:MET:HE3	1:24:A:ASN:HA	3	0.21	0.07	0.18
(1,138)	1:7:A:ASN:HB2	1:45:A:THR:HA	3	0.19	0.1	0.13
(1,138)	1:7:A:ASN:HB3	1:45:A:THR:HA	3	0.19	0.1	0.13
(1,139)	1:7:A:ASN:HB2	1:45:A:THR:HA	3	0.19	0.1	0.13
(1,139)	1:7:A:ASN:HB3	1:45:A:THR:HA	3	0.19	0.1	0.13
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG2	3	0.18	0.02	0.18
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG3	3	0.18	0.02	0.18
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	3	0.17	0.04	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	3	0.17	0.04	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	3	0.17	0.04	0.16
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	3	0.16	0.02	0.16
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	3	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	3	0.16	0.02	0.16
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	3	0.16	0.02	0.16
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD1	3	0.13	0.01	0.13
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD2	3	0.13	0.01	0.13
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG12	3	0.12	0.01	0.12
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG13	3	0.12	0.01	0.12
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG12	3	0.12	0.01	0.12
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG13	3	0.12	0.01	0.12
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD11	3	0.11	0.0	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD12	3	0.11	0.0	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD13	3	0.11	0.0	0.11
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	0.92	0.09	0.92
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	0.92	0.09	0.92
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	0.92	0.09	0.92
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	0.92	0.09	0.92
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA2	2	0.82	0.15	0.82
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA3	2	0.82	0.15	0.82
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA2	2	0.82	0.15	0.82
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA3	2	0.82	0.15	0.82
(1,224)	1:16:A:ARG:H	1:17:A:LYS:H	2	0.72	0.57	0.72
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG2	2	0.51	0.05	0.51
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG3	2	0.51	0.05	0.51
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	2	0.5	0.02	0.5
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE3	2	0.5	0.02	0.5
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	2	0.5	0.02	0.5
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE3	2	0.5	0.02	0.5
(1,149)	1:7:A:ASN:HD21	1:46:A:GLU:H	2	0.48	0.05	0.48
(1,149)	1:7:A:ASN:HD22	1:46:A:GLU:H	2	0.48	0.05	0.48
(1,150)	1:7:A:ASN:HD21	1:46:A:GLU:H	2	0.48	0.05	0.48
(1,150)	1:7:A:ASN:HD22	1:46:A:GLU:H	2	0.48	0.05	0.48
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	2	0.45	0.12	0.45
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	2	0.45	0.12	0.45
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	2	0.45	0.12	0.45
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	2	0.45	0.12	0.45
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	2	0.45	0.12	0.45
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	2	0.45	0.12	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	2	0.45	0.12	0.45
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	2	0.45	0.12	0.45
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	2	0.45	0.12	0.45
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	2	0.45	0.12	0.45
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	2	0.45	0.12	0.45
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	2	0.45	0.12	0.45
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD11	2	0.44	0.11	0.44
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD12	2	0.44	0.11	0.44
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD13	2	0.44	0.11	0.44
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD11	2	0.44	0.11	0.44
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD12	2	0.44	0.11	0.44
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD13	2	0.44	0.11	0.44
(1,1372)	1:78:A:VAL:HG11	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1372)	1:78:A:VAL:HG12	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1372)	1:78:A:VAL:HG13	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1372)	1:78:A:VAL:HG21	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1372)	1:78:A:VAL:HG22	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1372)	1:78:A:VAL:HG23	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG11	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG12	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG13	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG21	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG22	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1373)	1:78:A:VAL:HG23	1:79:A:GLU:H	2	0.39	0.12	0.39
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG11	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG12	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG13	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG21	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG22	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG23	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG11	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG12	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG13	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG21	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG22	2	0.36	0.1	0.36
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG23	2	0.36	0.1	0.36
(1,143)	1:7:A:ASN:HB2	1:46:A:GLU:H	2	0.34	0.1	0.34
(1,143)	1:7:A:ASN:HB3	1:46:A:GLU:H	2	0.34	0.1	0.34
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD21	2	0.34	0.23	0.34
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD22	2	0.34	0.23	0.34
(1,545)	1:34:A:THR:HG21	1:40:A:CYS:H	2	0.32	0.1	0.32
(1,545)	1:34:A:THR:HG22	1:40:A:CYS:H	2	0.32	0.1	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,545)	1:34:A:THR:HG23	1:40:A:CYS:H	2	0.32	0.1	0.32
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG21	2	0.32	0.12	0.32
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG22	2	0.32	0.12	0.32
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG23	2	0.32	0.12	0.32
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG2	2	0.32	0.2	0.32
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG3	2	0.32	0.2	0.32
(1,1307)	1:75:A:TYR:H	1:92:A:TRP:HZ3	2	0.32	0.12	0.32
(1,558)	1:36:A:ASN:HB2	1:37:A:CYS:H	2	0.31	0.02	0.31
(1,558)	1:36:A:ASN:HB3	1:37:A:CYS:H	2	0.31	0.02	0.31
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB2	2	0.3	0.08	0.3
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB3	2	0.3	0.08	0.3
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB2	2	0.3	0.08	0.3
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB3	2	0.3	0.08	0.3
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB2	2	0.3	0.16	0.3
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB3	2	0.3	0.16	0.3
(1,351)	1:26:A:HIS:HD2	1:32:A:TRP:HE3	2	0.28	0.12	0.28
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	0.24	0.08	0.24
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	0.24	0.08	0.24
(1,291)	1:20:A:ASP:HB2	1:32:A:TRP:HE1	2	0.24	0.06	0.24
(1,291)	1:20:A:ASP:HB3	1:32:A:TRP:HE1	2	0.24	0.06	0.24
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	2	0.22	0.05	0.22
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	2	0.22	0.05	0.22
(1,1470)	1:87:A:CYS:HB2	1:88:A:SER:H	2	0.22	0.04	0.22
(1,1470)	1:87:A:CYS:HB3	1:88:A:SER:H	2	0.22	0.04	0.22
(1,1471)	1:87:A:CYS:HB2	1:88:A:SER:H	2	0.22	0.04	0.22
(1,1471)	1:87:A:CYS:HB3	1:88:A:SER:H	2	0.22	0.04	0.22
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	2	0.21	0.11	0.21
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	2	0.21	0.11	0.21
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	2	0.21	0.11	0.21
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	2	0.21	0.11	0.21
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	2	0.21	0.11	0.21
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	2	0.21	0.11	0.21
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	2	0.21	0.11	0.21
(1,169)	1:8:A:GLU:H	1:9:A:GLY:H	2	0.2	0.09	0.2
(1,290)	1:20:A:ASP:HB2	1:32:A:TRP:HD1	2	0.19	0.08	0.19
(1,290)	1:20:A:ASP:HB3	1:32:A:TRP:HD1	2	0.19	0.08	0.19
(1,526)	1:33:A:GLN:HG2	1:34:A:THR:H	2	0.19	0.01	0.19

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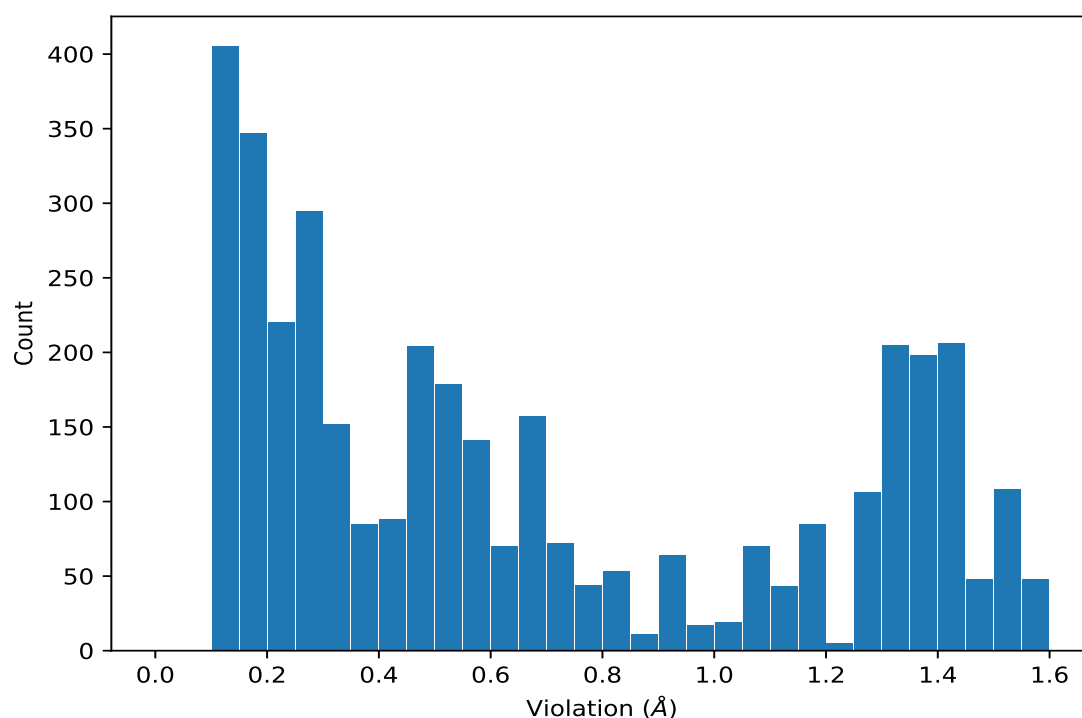
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,526)	1:33:A:GLN:HG3	1:34:A:THR:H	2	0.19	0.01	0.19
(1,527)	1:33:A:GLN:HG2	1:34:A:THR:H	2	0.19	0.01	0.19
(1,527)	1:33:A:GLN:HG3	1:34:A:THR:H	2	0.19	0.01	0.19
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE2	2	0.18	0.02	0.18
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE3	2	0.18	0.02	0.18
(1,145)	1:7:A:ASN:HB2	1:47:A:ILE:HG13	2	0.17	0.04	0.17
(1,145)	1:7:A:ASN:HB3	1:47:A:ILE:HG13	2	0.17	0.04	0.17
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD2	2	0.16	0.03	0.16
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD3	2	0.16	0.03	0.16
(1,35)	1:3:A:TYR:HD1	1:4:A:PHE:HA	2	0.15	0.02	0.15
(1,35)	1:3:A:TYR:HD2	1:4:A:PHE:HA	2	0.15	0.02	0.15
(1,318)	1:22:A:LYS:HB2	1:24:A:ASN:H	2	0.14	0.02	0.14
(1,318)	1:22:A:LYS:HB3	1:24:A:ASN:H	2	0.14	0.02	0.14
(1,319)	1:22:A:LYS:HB2	1:24:A:ASN:H	2	0.14	0.02	0.14
(1,319)	1:22:A:LYS:HB3	1:24:A:ASN:H	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG21	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG22	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG23	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG21	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG22	2	0.14	0.02	0.14
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG23	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG21	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG22	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG23	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG21	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG22	2	0.14	0.02	0.14
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG23	2	0.14	0.02	0.14

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	7	1.57
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	7	1.57
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	7	1.57
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	7	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	7	1.57
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	7	1.57
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	7	1.57
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	7	1.57
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	7	1.57
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	7	1.57
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	7	1.57
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	7	1.57
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	7	1.57
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.54
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.54
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.54
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.54
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.54
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.54
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.54
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.54
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.54
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	10	1.54
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	10	1.54
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	10	1.54
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	1	1.53
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	1	1.53
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	1	1.53
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	1	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	1	1.53
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	1	1.53
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	1	1.53
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	1	1.53
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	1	1.53
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	1	1.53
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	1	1.53
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	1	1.53
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	9	1.52
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	9	1.52
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	9	1.52
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	9	1.52
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	9	1.52
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	9	1.52
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	9	1.52
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	9	1.52
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	9	1.52
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	9	1.52
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	9	1.52
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	9	1.52
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	9	1.52
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	9	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	9	1.52
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	9	1.52
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	9	1.52
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	9	1.52
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	6	1.49
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	6	1.49
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	6	1.49
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	6	1.49
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	6	1.49
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	6	1.49
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	6	1.49
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	6	1.49
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	6	1.49
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	6	1.49
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	6	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	6	1.49
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	6	1.49
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	6	1.49
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	6	1.49
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	6	1.49
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	6	1.49
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	6	1.49
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	2	1.44
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	2	1.44
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	2	1.44
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	2	1.44
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	2	1.44
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	2	1.44
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	2	1.44
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	2	1.44
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	2	1.44
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	2	1.44
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	2	1.44
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	2	1.44
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	2	1.44
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	2	1.44
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	2	1.44
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	2	1.44
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	2	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	2	1.44
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	2	1.44
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	2	1.44
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	2	1.44
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	2	1.44
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	2	1.44
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	2	1.44
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	2	1.44
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	5	1.42
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	5	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	5	1.42
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	5	1.42
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	5	1.42
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	5	1.42
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	5	1.42
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	8	1.42
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	8	1.42
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	8	1.42
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	8	1.42
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	8	1.42
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	8	1.42
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	8	1.42
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	5	1.42
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	5	1.42
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	8	1.42
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	8	1.42
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	8	1.42
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	8	1.42
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	8	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	8	1.42
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	5	1.42
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	5	1.42
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	8	1.42
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	8	1.42
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	8	1.42
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	5	1.42
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	5	1.42
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	8	1.42
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	8	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	8	1.42
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	8	1.42
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	8	1.42
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	8	1.42
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	8	1.42
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	9	1.42
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	9	1.42
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	9	1.42
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	9	1.42
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	9	1.42
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	9	1.42
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	9	1.42
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	9	1.42
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	9	1.42
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	9	1.42
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	9	1.42
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	9	1.42
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	9	1.42
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	9	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	9	1.42
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	9	1.42
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	9	1.42
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	9	1.42
(1,1241)	1:70:A:LYS:HG2	1:71:A:GLU:H	4	1.41
(1,1241)	1:70:A:LYS:HG3	1:71:A:GLU:H	4	1.41
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	3	1.39
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	3	1.39
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	3	1.39
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	3	1.39
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	3	1.39
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	3	1.39
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	3	1.39
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	3	1.39
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	3	1.39
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	3	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	3	1.39
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	3	1.39
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	3	1.39
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	3	1.39
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	3	1.39
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	3	1.39
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	3	1.39
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	3	1.39
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	7	1.39
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	7	1.39
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	7	1.39
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	7	1.39
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	7	1.39
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	7	1.39
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	7	1.39
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD11	2	1.39
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD12	2	1.39
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD13	2	1.39
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	4	1.38
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	4	1.38
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	4	1.38
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	4	1.38
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	4	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	4	1.38
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	4	1.38
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	4	1.38
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	4	1.38
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	4	1.38
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	4	1.38
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	4	1.38
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	4	1.38
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	4	1.38
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	4	1.38
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	4	1.38
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	4	1.38
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	4	1.38
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	4	1.38
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	4	1.38
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	4	1.38
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	4	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	4	1.38
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	8	1.38
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	8	1.38
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	8	1.38
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	8	1.38
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	8	1.38
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	8	1.38
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	8	1.38
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.37
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.37
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.37
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.37
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.37
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.37
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.37
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.37
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.37
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.37
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.37
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.37
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.37
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.37
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	10	1.37
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	10	1.37
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	10	1.37
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	5	1.37
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	5	1.37
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	5	1.37
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	10	1.36
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	10	1.36
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	4	1.35
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	4	1.35
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	4	1.35
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	4	1.35
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	4	1.35
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	4	1.35
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	4	1.35
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	4	1.35
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	4	1.35
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	4	1.35
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	4	1.35
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	4	1.33
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	4	1.33
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	4	1.33
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	4	1.33
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	4	1.33
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	4	1.33
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	4	1.33
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	4	1.33
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	4	1.33
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	4	1.33
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	4	1.33
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	4	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	4	1.33
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	4	1.33
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	4	1.33
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	4	1.33
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	4	1.33
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	4	1.33
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	1	1.32
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	1	1.32
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	1	1.32
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	1	1.32
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	1	1.32
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	1	1.32
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	1	1.32
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	1	1.32
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	1	1.32
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	1	1.32
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	1	1.32
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	1	1.32
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	1	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	1	1.32
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	1	1.32
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	1	1.32
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	1	1.32
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	1	1.32
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	1	1.32
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	1	1.32
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	7	1.32
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	7	1.32
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	7	1.32
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	7	1.32
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	7	1.32
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	7	1.32
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	1	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	1	1.32
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	1	1.32
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	1	1.32
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	1	1.32
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	1	1.32
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	1	1.32
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	7	1.32
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	7	1.32
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	7	1.32
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	1	1.32
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	1	1.32
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	7	1.32
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	7	1.32
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	7	1.32
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	7	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	7	1.32
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	7	1.32
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	1	1.32
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	1	1.32
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	7	1.32
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	7	1.32
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	7	1.32
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	8	1.32
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	5	1.3
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	5	1.3
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	5	1.3
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	5	1.3
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	5	1.3
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	5	1.3
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	5	1.3
(1,224)	1:16:A:ARG:H	1:17:A:LYS:H	10	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	8	1.29
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	8	1.29
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	8	1.29
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	8	1.29
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	8	1.29
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	8	1.29
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	8	1.29
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	8	1.29
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	8	1.29
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	8	1.29
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	8	1.29
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	8	1.29
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	8	1.29
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	8	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	8	1.29
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	8	1.29
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	8	1.29
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	8	1.29
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	2	1.27
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	2	1.27
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	2	1.27
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	2	1.27
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	2	1.27
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	2	1.27
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	2	1.27
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	2	1.27
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	2	1.27
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	2	1.27
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	2	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	2	1.27
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	2	1.27
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	2	1.27
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	2	1.27
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	2	1.27
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	2	1.27
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	2	1.27
(1,762)	1:51:A:THR:HG21	1:53:A:VAL:HB	10	1.26
(1,762)	1:51:A:THR:HG22	1:53:A:VAL:HB	10	1.26
(1,762)	1:51:A:THR:HG23	1:53:A:VAL:HB	10	1.26
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	2	1.26
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	2	1.26
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	2	1.26
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	9	1.26
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	9	1.26
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	9	1.26
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	10	1.24
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	1	1.23
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	1	1.23
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	5	1.22
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	5	1.22
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	8	1.19
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	8	1.19
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	8	1.19
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	8	1.19
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	8	1.19
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	8	1.19
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	8	1.19
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	8	1.19
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	8	1.19
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	8	1.19
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	8	1.19
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	8	1.19
(1,762)	1:51:A:THR:HG21	1:53:A:VAL:HB	7	1.19
(1,762)	1:51:A:THR:HG22	1:53:A:VAL:HB	7	1.19
(1,762)	1:51:A:THR:HG23	1:53:A:VAL:HB	7	1.19
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	3	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	3	1.19
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	3	1.18
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	3	1.18
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	3	1.18
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	3	1.18
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	3	1.18
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	3	1.18
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	3	1.18
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	3	1.18
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	3	1.18
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	3	1.18
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	3	1.18
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	3	1.18
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	3	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	3	1.18
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	3	1.18
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	3	1.18
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	3	1.18
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	3	1.18
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	6	1.16
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	6	1.16
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	10	1.16
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	10	1.16
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	10	1.16
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	10	1.16
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	10	1.16
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	10	1.16
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	10	1.16
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	10	1.16
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	10	1.16
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	10	1.16
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	10	1.16
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	10	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	2	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	2	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	2	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	2	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	2	1.16
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	2	1.16
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	4	1.15
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	4	1.15
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	4	1.15
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	4	1.15
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	4	1.15
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	4	1.15
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	8	1.15
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	8	1.15
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	8	1.15
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	7	1.13
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	7	1.13
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	10	1.13
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	10	1.13
(1,560)	1:36:A:ASN:HB2	1:37:A:CYS:H	10	1.13
(1,560)	1:36:A:ASN:HB3	1:37:A:CYS:H	10	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:36:A:ASN:HB2	1:37:A:CYS:H	10	1.13
(1,559)	1:36:A:ASN:HB3	1:37:A:CYS:H	10	1.13
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	9	1.12
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	9	1.12
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	3	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	10	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	10	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	10	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	10	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	10	1.11
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	10	1.11
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	4	1.1
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	4	1.1
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	4	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	4	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	4	1.1
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	4	1.1
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	4	1.1
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	4	1.1
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	4	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	4	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	4	1.1
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	4	1.1
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	2	1.1
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	2	1.1
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	2	1.1
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	2	1.1
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	3	1.1
(1,560)	1:36:A:ASN:HB2	1:37:A:CYS:H	2	1.09
(1,560)	1:36:A:ASN:HB3	1:37:A:CYS:H	2	1.09
(1,559)	1:36:A:ASN:HB2	1:37:A:CYS:H	2	1.09
(1,559)	1:36:A:ASN:HB3	1:37:A:CYS:H	2	1.09
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	9	1.09
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	6	1.08
(1,1342)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	6	1.08
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	6	1.08
(1,1342)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	6	1.08
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	6	1.08
(1,1342)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	6	1.08
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	6	1.08
(1,1342)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	6	1.08
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	6	1.08
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	6	1.08
(1,1342)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	6	1.08
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	6	1.08
(1,1341)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	6	1.08
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	6	1.08
(1,1340)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG11	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG12	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG13	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG21	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG22	1:87:A:CYS:HB3	6	1.08
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB2	6	1.08
(1,1339)	1:77:A:VAL:HG23	1:87:A:CYS:HB3	6	1.08
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	10	1.06
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	10	1.06
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	10	1.06
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	10	1.06
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	10	1.06
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	10	1.06
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	10	1.06
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	10	1.06
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	10	1.06
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	10	1.06
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	10	1.06
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE2	6	1.05
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE3	6	1.05
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE2	6	1.05
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE3	6	1.05
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	1	1.05
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE2	8	1.04
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE3	8	1.04
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE2	8	1.04
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE3	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	8	1.04
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	8	1.04
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE2	1	1.03
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE3	1	1.03
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE2	1	1.03
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE3	1	1.03
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	1.01
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	1.01
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	1.01
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	1.01
(1,231)	1:17:A:LYS:H	1:18:A:CYS:H	3	1.0
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	4	0.98
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA2	2	0.97
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA3	2	0.97
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA2	2	0.97
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA3	2	0.97
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	9	0.96
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	9	0.96
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	9	0.96
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	9	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	9	0.96
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	9	0.96
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	9	0.96
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	6	0.95
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	6	0.95
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	6	0.95
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	6	0.95
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	6	0.95
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	6	0.95
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	1	0.95
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	1	0.95
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	1	0.95
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	1	0.95
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	1	0.95
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	1	0.95
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	4	0.94
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	4	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	4	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	4	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	4	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	4	0.94
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	8	0.94
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	8	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	8	0.94
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	8	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	8	0.94
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	8	0.94
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	7	0.93
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	7	0.93
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	7	0.93
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	7	0.93
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	7	0.93
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	7	0.93
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	7	0.93
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	7	0.93
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	7	0.93
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	7	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	7	0.93
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	7	0.93
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	7	0.93
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	7	0.93
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	7	0.93
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	7	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	3	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	3	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	3	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	3	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	3	0.93
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	3	0.93
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	3	0.92
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	3	0.92
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	3	0.92
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	3	0.92
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	3	0.92
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	3	0.92
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE2	9	0.91
(1,1157)	1:67:A:ILE:HG21	1:69:A:LYS:HE3	9	0.91
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE2	9	0.91
(1,1157)	1:67:A:ILE:HG22	1:69:A:LYS:HE3	9	0.91
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE2	9	0.91
(1,1157)	1:67:A:ILE:HG23	1:69:A:LYS:HE3	9	0.91
(1,522)	1:33:A:GLN:HE21	1:39:A:THR:HG21	5	0.91
(1,522)	1:33:A:GLN:HE21	1:39:A:THR:HG22	5	0.91
(1,522)	1:33:A:GLN:HE21	1:39:A:THR:HG23	5	0.91
(1,522)	1:33:A:GLN:HE22	1:39:A:THR:HG21	5	0.91
(1,522)	1:33:A:GLN:HE22	1:39:A:THR:HG22	5	0.91
(1,522)	1:33:A:GLN:HE22	1:39:A:THR:HG23	5	0.91
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	7	0.88
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	7	0.88
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	7	0.88
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	7	0.88
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE2	3	0.87
(1,1447)	1:84:A:LYS:HB2	1:84:A:LYS:HE3	3	0.87
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE2	3	0.87
(1,1447)	1:84:A:LYS:HB3	1:84:A:LYS:HE3	3	0.87
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD11	4	0.86
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD12	4	0.86
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD13	4	0.86
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD11	3	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD12	3	0.85
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD13	3	0.85
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	7	0.85
(1,762)	1:51:A:THR:HG21	1:53:A:VAL:HB	4	0.84
(1,762)	1:51:A:THR:HG22	1:53:A:VAL:HB	4	0.84
(1,762)	1:51:A:THR:HG23	1:53:A:VAL:HB	4	0.84
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD11	4	0.84
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD12	4	0.84
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD13	4	0.84
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	10	0.84
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	10	0.84
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	10	0.84
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	10	0.84
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB2	6	0.84
(1,183)	1:10:A:VAL:HB	1:13:A:ASP:HB3	6	0.84
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB2	6	0.84
(1,182)	1:10:A:VAL:HB	1:13:A:ASP:HB3	6	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	1	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	1	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	1	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	1	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	1	0.84
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	1	0.84
(1,472)	1:32:A:TRP:HD1	1:34:A:THR:HB	7	0.83
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD11	1	0.83
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD12	1	0.83
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD13	1	0.83
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	1	0.82
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	1	0.82
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	1	0.82
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	1	0.82
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	1	0.82
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	1	0.82
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	1	0.82
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	1	0.82
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	1	0.82
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	1	0.82
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	1	0.82
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	1	0.82
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	1	0.81
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	1	0.81
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	1	0.81
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	1	0.81
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	1	0.81
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	4	0.81
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	4	0.81
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	4	0.81
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	8	0.8
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	8	0.8
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	8	0.8
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	8	0.8
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	10	0.79
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	2	0.79
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	2	0.79
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	2	0.79
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	2	0.79
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	2	0.79
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	2	0.79
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	2	0.78
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	2	0.78
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	2	0.78
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	2	0.78
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	2	0.78
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	2	0.78
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	2	0.78
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	2	0.78
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	2	0.78
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	2	0.78
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	2	0.78
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	2	0.78
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	3	0.78
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	4	0.78
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	5	0.78
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	8	0.78
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD21	8	0.78
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	8	0.78
(1,335)	1:24:A:ASN:H	1:24:A:ASN:HD21	8	0.78
(1,335)	1:24:A:ASN:H	1:24:A:ASN:HD22	8	0.78
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	5	0.76
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	5	0.76
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	5	0.76
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	5	0.76
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	5	0.76
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	5	0.76
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	5	0.76
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	5	0.76
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	5	0.76
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	5	0.76
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	5	0.76
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	6	0.76
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	6	0.76
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	6	0.76
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	6	0.76
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	9	0.75
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	6	0.74
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	6	0.74
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	6	0.74
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	7	0.74
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	7	0.74
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	7	0.74
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	5	0.73
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	5	0.73
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	5	0.73
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	5	0.73
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	3	0.72
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	3	0.72
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	3	0.72
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	3	0.72
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	3	0.72
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	3	0.72
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	3	0.72
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	3	0.72
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	3	0.72
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	3	0.72
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	3	0.72
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	3	0.72
(1,714)	1:45:A:THR:HG21	1:46:A:GLU:H	2	0.72
(1,714)	1:45:A:THR:HG22	1:46:A:GLU:H	2	0.72
(1,714)	1:45:A:THR:HG23	1:46:A:GLU:H	2	0.72
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	9	0.72
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	9	0.72
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	9	0.72
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	9	0.72
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	9	0.72
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	9	0.72
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	9	0.72
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	9	0.72
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	9	0.72
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	2	0.72
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	2	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	4	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	4	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	4	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	6	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	6	0.72
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	6	0.72
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD11	2	0.72
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD12	2	0.72
(1,83)	1:5:A:ILE:HA	1:5:A:ILE:HD13	2	0.72
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	9	0.71
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	9	0.71
(1,1091)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	9	0.71
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	9	0.71
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	9	0.71
(1,1091)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	9	0.71
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	9	0.71
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	9	0.71
(1,1090)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	9	0.71
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	9	0.71
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	9	0.71
(1,1090)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	9	0.71
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE1	3	0.71
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE2	3	0.71
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	7	0.71
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	7	0.71
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	7	0.71
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	7	0.71
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	7	0.71
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	7	0.71
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	7	0.71
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	7	0.71
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	7	0.71
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	7	0.71
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	7	0.71
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	10	0.7
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	10	0.7
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	10	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	10	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	10	0.7
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	10	0.7
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	10	0.7
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	10	0.7
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	10	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	10	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	10	0.7
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	10	0.7
(1,135)	1:7:A:ASN:HA	1:47:A:ILE:HG13	4	0.7
(1,28)	1:2:A:CYS:H	1:50:A:CYS:HA	5	0.7
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD11	10	0.69
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD12	10	0.69
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD13	10	0.69
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	8	0.69
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	8	0.69
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	8	0.69
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	8	0.69
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	8	0.69
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	8	0.69
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	8	0.69
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	8	0.69
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	8	0.69
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	8	0.69
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	8	0.69
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	8	0.69
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	6	0.69
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	6	0.69
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	6	0.69
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	6	0.69
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	10	0.69
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	10	0.69
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	10	0.69
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	10	0.69
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	10	0.69
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	10	0.69
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	10	0.69
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	10	0.69
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	10	0.69
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	10	0.69
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	10	0.69
(1,203)	1:12:A:GLY:H	1:13:A:ASP:H	10	0.69
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	9	0.69
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	9	0.69
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	9	0.69
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	9	0.69
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	7	0.68
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	2	0.68
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	2	0.68
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	2	0.68
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	2	0.68
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	2	0.68
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	2	0.68
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	2	0.68
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	2	0.68
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	9	0.68
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	9	0.68
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	9	0.68
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	9	0.68
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	9	0.68
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	9	0.68
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	9	0.68
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	9	0.68
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	9	0.68
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	9	0.68
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	9	0.68
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	9	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	6	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	6	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	6	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	6	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	6	0.68
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	6	0.68
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	5	0.67
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	5	0.67
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	5	0.67
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	5	0.67
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	5	0.67
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	5	0.67
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	5	0.67
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	5	0.67
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	5	0.67
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	5	0.67
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	5	0.67
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	6	0.67
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	2	0.67
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	2	0.67
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	2	0.67
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	2	0.67
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	2	0.67
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	2	0.67
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	2	0.67
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	2	0.67
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	2	0.67
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	2	0.67
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	2	0.67
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	2	0.67
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	3	0.67
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	3	0.67
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	3	0.67
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	3	0.67
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA2	10	0.67
(1,132)	1:6:A:PRO:HG2	1:9:A:GLY:HA3	10	0.67
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA2	10	0.67
(1,132)	1:6:A:PRO:HG3	1:9:A:GLY:HA3	10	0.67
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	5	0.66
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	5	0.66
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	5	0.66
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	5	0.66
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	5	0.66
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	5	0.66
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	5	0.66
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	5	0.66
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	5	0.66
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	5	0.66
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	5	0.66
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	8	0.65
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	8	0.65
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	8	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	8	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	8	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	8	0.65
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	9	0.65
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	9	0.65
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	9	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	9	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	9	0.65
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	9	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	8	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	8	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	8	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	8	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	8	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	8	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	9	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	9	0.65
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	9	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	9	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	9	0.65
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	9	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	8	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	8	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	8	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	8	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	8	0.65
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	8	0.65
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	6	0.64
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	10	0.64
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	1	0.64
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	1	0.64
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	9	0.64
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	9	0.64
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	9	0.64
(1,157)	1:7:A:ASN:H	1:7:A:ASN:HD21	7	0.64
(1,157)	1:7:A:ASN:H	1:7:A:ASN:HD22	7	0.64
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	3	0.63
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	3	0.63
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	3	0.63
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	3	0.63
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	3	0.63
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	6	0.63
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	6	0.63
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	6	0.63
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	6	0.63
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	6	0.63
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	6	0.63
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	6	0.63
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	6	0.63
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	6	0.63
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	6	0.63
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	6	0.63
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	6	0.63
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	5	0.63
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	5	0.63
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	5	0.63
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	6	0.63
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	6	0.63
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	6	0.63
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	6	0.62
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	6	0.62
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	6	0.62
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	6	0.62
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	6	0.62
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	6	0.62
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	6	0.62
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	6	0.62
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	6	0.62
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	6	0.62
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	6	0.62
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	6	0.62
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	8	0.62
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	8	0.62
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	8	0.62
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	8	0.62
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	8	0.62
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	8	0.62
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	1	0.62
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG21	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG22	2	0.62
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG23	2	0.62
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG21	2	0.62
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG22	2	0.62
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG23	2	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	9	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	9	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	9	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	9	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	9	0.62
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	9	0.62
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	3	0.61
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	3	0.61
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	7	0.61
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	7	0.61
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	6	0.61
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	6	0.61
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	2	0.6
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	2	0.6
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	9	0.6
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	9	0.6
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	9	0.6
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	9	0.6
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	9	0.6
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	6	0.59
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	6	0.59
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	1	0.59
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	1	0.59
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	1	0.59
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	1	0.59
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	1	0.59
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	1	0.59
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG21	3	0.59
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG22	3	0.59
(1,535)	1:33:A:GLN:HG2	1:39:A:THR:HG23	3	0.59
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG21	3	0.59
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG22	3	0.59
(1,535)	1:33:A:GLN:HG3	1:39:A:THR:HG23	3	0.59
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG21	3	0.59
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG22	3	0.59
(1,534)	1:33:A:GLN:HG2	1:39:A:THR:HG23	3	0.59
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG21	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG22	3	0.59
(1,534)	1:33:A:GLN:HG3	1:39:A:THR:HG23	3	0.59
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	7	0.59
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	7	0.59
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	7	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	3	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	3	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	5	0.59
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	5	0.59
(1,265)	1:19:A:MET:HE1	1:25:A:LYS:HA	9	0.59
(1,265)	1:19:A:MET:HE2	1:25:A:LYS:HA	9	0.59
(1,265)	1:19:A:MET:HE3	1:25:A:LYS:HA	9	0.59
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	8	0.58
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	8	0.58
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	9	0.58
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	9	0.58
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	9	0.58
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	9	0.58
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	9	0.58
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	9	0.58
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	9	0.58
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	9	0.58
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	9	0.58
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	9	0.58
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	9	0.58
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	9	0.58
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	9	0.58
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	10	0.58
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	10	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	3	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	3	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	3	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	3	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	3	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	3	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	6	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	6	0.58
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	6	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	6	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	6	0.58
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	6	0.58
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	3	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	3	0.58
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	3	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	3	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	3	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	3	0.58
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	6	0.58
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	6	0.58
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	6	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	6	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	6	0.58
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	6	0.58
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	3	0.58
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	3	0.58
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	3	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	4	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	4	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	4	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	4	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	4	0.58
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	4	0.58
(1,135)	1:7:A:ASN:HA	1:47:A:ILE:HG13	9	0.58
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE2	8	0.57
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE3	8	0.57
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE2	8	0.57
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE3	8	0.57
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG2	5	0.56
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG3	5	0.56
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	9	0.56
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	9	0.56
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	9	0.56
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	9	0.56
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	9	0.56
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	9	0.56
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	6	0.56
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	6	0.56
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	6	0.56
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	6	0.56
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	3	0.56
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	3	0.56
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	3	0.56
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	3	0.56
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	4	0.56
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	4	0.56
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	4	0.56
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	4	0.56
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	4	0.56
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	4	0.56
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	4	0.56
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	4	0.56
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	4	0.56
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	4	0.56
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	4	0.56
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD21	1	0.56
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD22	1	0.56
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	2	0.56
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	2	0.56
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	2	0.56
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	4	0.56
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	4	0.56
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	4	0.56
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	4	0.56
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	8	0.56
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	8	0.56
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB2	5	0.56
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB3	5	0.56
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB2	5	0.56
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB3	5	0.56
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB2	5	0.56
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB3	5	0.56
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	7	0.55
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	5	0.55
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	5	0.55
(1,256)	1:19:A:MET:HA	1:26:A:HIS:HD2	9	0.55
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD11	9	0.54
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD12	9	0.54
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD13	9	0.54
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD11	9	0.54
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD12	9	0.54
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD13	9	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	6	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	6	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	6	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	6	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	6	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	8	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	8	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	8	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	8	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	8	0.54
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	6	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	8	0.54
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	8	0.54
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	6	0.54
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	6	0.54
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	6	0.54
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	6	0.54
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	6	0.54
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	6	0.54
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD11	9	0.54
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD12	9	0.54
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD13	9	0.54
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	8	0.54
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	8	0.54
(1,407)	1:28:A:ILE:HG21	1:29:A:ASN:HB2	1	0.54
(1,407)	1:28:A:ILE:HG22	1:29:A:ASN:HB2	1	0.54
(1,407)	1:28:A:ILE:HG23	1:29:A:ASN:HB2	1	0.54
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	3	0.54
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	3	0.54
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	3	0.54
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	3	0.54
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	4	0.54
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	4	0.54
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	10	0.54
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	10	0.54
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	10	0.54
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	10	0.54
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	10	0.54
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE2	5	0.54
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE3	5	0.54
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE2	5	0.54
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE3	5	0.54
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	6	0.54
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	6	0.54
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	6	0.54
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	6	0.54
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	6	0.54
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	6	0.54
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	9	0.54
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	9	0.54
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	9	0.54
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	9	0.54
(1,1240)	1:70:A:LYS:HG2	1:71:A:GLU:HA	4	0.53
(1,1240)	1:70:A:LYS:HG3	1:71:A:GLU:HA	4	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	10	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	10	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	10	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	10	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	10	0.53
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	10	0.53
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	10	0.53
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	5	0.53
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	5	0.53
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	10	0.53
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	10	0.53
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	10	0.53
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	10	0.53
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	10	0.53
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	10	0.53
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	9	0.53
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	9	0.53
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	9	0.53
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	9	0.53
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	9	0.53
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	9	0.53
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	9	0.53
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG2	4	0.52
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG3	4	0.52
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE1	8	0.52
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE2	8	0.52
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE1	8	0.52
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE2	8	0.52
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	4	0.52
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	4	0.52
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	4	0.52
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	4	0.52
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG2	10	0.52
(1,325)	1:22:A:LYS:H	1:22:A:LYS:HG3	10	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD11	1	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD12	1	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD13	1	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD21	1	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD22	1	0.52
(1,308)	1:21:A:LEU:H	1:21:A:LEU:HD23	1	0.52
(1,150)	1:7:A:ASN:HD21	1:46:A:GLU:H	10	0.52
(1,150)	1:7:A:ASN:HD22	1:46:A:GLU:H	10	0.52
(1,149)	1:7:A:ASN:HD21	1:46:A:GLU:H	10	0.52
(1,149)	1:7:A:ASN:HD22	1:46:A:GLU:H	10	0.52
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	2	0.51
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE3	2	0.51
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	2	0.51
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE3	2	0.51
(1,1373)	1:78:A:VAL:HG11	1:79:A:GLU:H	9	0.51
(1,1373)	1:78:A:VAL:HG12	1:79:A:GLU:H	9	0.51
(1,1373)	1:78:A:VAL:HG13	1:79:A:GLU:H	9	0.51
(1,1373)	1:78:A:VAL:HG21	1:79:A:GLU:H	9	0.51
(1,1373)	1:78:A:VAL:HG22	1:79:A:GLU:H	9	0.51
(1,1373)	1:78:A:VAL:HG23	1:79:A:GLU:H	9	0.51
(1,1372)	1:78:A:VAL:HG11	1:79:A:GLU:H	9	0.51
(1,1372)	1:78:A:VAL:HG12	1:79:A:GLU:H	9	0.51
(1,1372)	1:78:A:VAL:HG13	1:79:A:GLU:H	9	0.51
(1,1372)	1:78:A:VAL:HG21	1:79:A:GLU:H	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:78:A:VAL:HG22	1:79:A:GLU:H	9	0.51
(1,1372)	1:78:A:VAL:HG23	1:79:A:GLU:H	9	0.51
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE1	10	0.51
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE2	10	0.51
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE1	10	0.51
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE2	10	0.51
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	3	0.51
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	3	0.51
(1,223)	1:16:A:ARG:H	1:16:A:ARG:HG2	2	0.51
(1,223)	1:16:A:ARG:H	1:16:A:ARG:HG3	2	0.51
(1,163)	1:8:A:GLU:HB2	1:9:A:GLY:H	6	0.51
(1,163)	1:8:A:GLU:HB3	1:9:A:GLY:H	6	0.51
(1,162)	1:8:A:GLU:HB2	1:9:A:GLY:H	6	0.51
(1,162)	1:8:A:GLU:HB3	1:9:A:GLY:H	6	0.51
(1,1424)	1:81:A:LYS:H	1:81:A:LYS:HG2	2	0.5
(1,1424)	1:81:A:LYS:H	1:81:A:LYS:HG3	2	0.5
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	4	0.5
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB2	4	0.5
(1,483)	1:32:A:TRP:HH2	1:42:A:CYS:HB3	4	0.5
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	2	0.5
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	2	0.5
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	2	0.5
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	2	0.5
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	1	0.5
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	1	0.5
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	1	0.5
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	1	0.5
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	1	0.5
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	1	0.5
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	1	0.5
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	1	0.5
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	1	0.5
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	1	0.5
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	1	0.5
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	1	0.5
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	2	0.5
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	2	0.5
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	2	0.5
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	2	0.5
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	2	0.5
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	2	0.5
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	2	0.5
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	1	0.49
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	1	0.49
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	1	0.49
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	1	0.49
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	1	0.49
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	1	0.49
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	1	0.49
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	2	0.49
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	2	0.49
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	5	0.49
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	7	0.49
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	7	0.49
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	7	0.49
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	7	0.49
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	10	0.49
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	10	0.49
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	10	0.49
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	1	0.49
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	1	0.49
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	1	0.49
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	1	0.49
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	1	0.49
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	1	0.49
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	1	0.49
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	1	0.49
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	1	0.48
(1,1419)	1:81:A:LYS:HB2	1:81:A:LYS:HE3	1	0.48
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	1	0.48
(1,1419)	1:81:A:LYS:HB3	1:81:A:LYS:HE3	1	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	2	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	4	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	4	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	4	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	4	0.48
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	2	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	4	0.48
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	4	0.48
(1,1094)	1:65:A:GLN:HE21	1:80:A:LYS:HA	3	0.48
(1,1094)	1:65:A:GLN:HE22	1:80:A:LYS:HA	3	0.48
(1,1093)	1:65:A:GLN:HE21	1:80:A:LYS:HA	3	0.48
(1,1093)	1:65:A:GLN:HE22	1:80:A:LYS:HA	3	0.48
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	4	0.48
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	4	0.48
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	7	0.48
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	7	0.48
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	10	0.48
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	10	0.48
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	7	0.48
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	7	0.48
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	10	0.48
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	10	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG11	7	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG12	7	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG13	7	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG21	7	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG22	7	0.48
(1,173)	1:9:A:GLY:H	1:10:A:VAL:HG23	7	0.48
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	1	0.48
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	1	0.48
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	1	0.48
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	4	0.47
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	4	0.47
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	4	0.47
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	4	0.47
(1,1288)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	4	0.47
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG21	4	0.47
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG22	4	0.47
(1,1287)	1:74:A:LYS:HE2	1:76:A:ILE:HG23	4	0.47
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG21	4	0.47
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG22	4	0.47
(1,1287)	1:74:A:LYS:HE3	1:76:A:ILE:HG23	4	0.47
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	8	0.47
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	8	0.47
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	8	0.47
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	8	0.47
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	8	0.47
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	8	0.47
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	4	0.47
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	4	0.47
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	4	0.47
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	4	0.47
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	4	0.47
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	4	0.47
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	6	0.47
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	6	0.47
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	6	0.47
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	6	0.47
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	6	0.47
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	6	0.47
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	6	0.47
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	6	0.47
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	6	0.47
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	6	0.47
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	6	0.47
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	6	0.47
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	5	0.47
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	5	0.47
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	5	0.47
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	5	0.47
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	5	0.47
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	5	0.47
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	10	0.47
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	10	0.47
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	10	0.47
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	10	0.47
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	10	0.47
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	10	0.47
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	10	0.47
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG2	3	0.46
(1,1075)	1:64:A:CYS:H	1:80:A:LYS:HG3	3	0.46
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	7	0.46
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	7	0.46
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD2	5	0.46
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD3	5	0.46
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	7	0.46
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	7	0.46
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	7	0.46
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	7	0.46
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	7	0.46
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	7	0.46
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB2	2	0.46
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB3	2	0.46
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG11	7	0.45
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG12	7	0.45
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG13	7	0.45
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG21	7	0.45
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG22	7	0.45
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG23	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG11	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG12	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG13	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG21	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG22	7	0.45
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG23	7	0.45
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	1	0.45
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	1	0.45
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	1	0.45
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	1	0.45
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	1	0.45
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	1	0.45
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	1	0.45
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	1	0.45
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	1	0.45
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	1	0.45
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	1	0.45
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	7	0.45
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	7	0.45
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	7	0.45
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	7	0.45
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	7	0.45
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	7	0.45
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG21	8	0.45
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG22	8	0.45
(1,456)	1:31:A:GLU:HG2	1:41:A:THR:HG23	8	0.45
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG21	8	0.45
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG22	8	0.45
(1,456)	1:31:A:GLU:HG3	1:41:A:THR:HG23	8	0.45
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG21	8	0.45
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG22	8	0.45
(1,455)	1:31:A:GLU:HG2	1:41:A:THR:HG23	8	0.45
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG21	8	0.45
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG22	8	0.45
(1,455)	1:31:A:GLU:HG3	1:41:A:THR:HG23	8	0.45
(1,203)	1:12:A:GLY:H	1:13:A:ASP:H	9	0.45
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	5	0.45
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	5	0.45
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	5	0.45
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	5	0.45
(1,135)	1:7:A:ASN:HA	1:47:A:ILE:HG13	6	0.45
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	3	0.45
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	3	0.45
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	3	0.45
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	3	0.45
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	3	0.45
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	3	0.45
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	3	0.45
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	3	0.45
(1,29)	1:2:A:CYS:H	1:51:A:THR:HG21	5	0.45
(1,29)	1:2:A:CYS:H	1:51:A:THR:HG22	5	0.45
(1,29)	1:2:A:CYS:H	1:51:A:THR:HG23	5	0.45
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	3	0.44
(1,508)	1:32:A:TRP:HZ3	1:42:A:CYS:H	1	0.44
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	4	0.44
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	4	0.44
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	4	0.44
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	7	0.44
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	7	0.44
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	7	0.44
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	7	0.44
(1,143)	1:7:A:ASN:HB2	1:46:A:GLU:H	6	0.44
(1,143)	1:7:A:ASN:HB3	1:46:A:GLU:H	6	0.44
(1,1307)	1:75:A:TYR:H	1:92:A:TRP:HZ3	8	0.43
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	2	0.43
(1,150)	1:7:A:ASN:HD21	1:46:A:GLU:H	7	0.43
(1,150)	1:7:A:ASN:HD22	1:46:A:GLU:H	7	0.43
(1,149)	1:7:A:ASN:HD21	1:46:A:GLU:H	7	0.43
(1,149)	1:7:A:ASN:HD22	1:46:A:GLU:H	7	0.43
(1,142)	1:7:A:ASN:HB2	1:46:A:GLU:HA	8	0.43
(1,142)	1:7:A:ASN:HB3	1:46:A:GLU:HA	8	0.43
(1,141)	1:7:A:ASN:HB2	1:46:A:GLU:HA	8	0.43
(1,141)	1:7:A:ASN:HB3	1:46:A:GLU:HA	8	0.43
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG21	9	0.43
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG22	9	0.43
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG23	9	0.43
(1,99)	1:5:A:ILE:HD11	1:11:A:PRO:HD2	10	0.43
(1,99)	1:5:A:ILE:HD12	1:11:A:PRO:HD2	10	0.43
(1,99)	1:5:A:ILE:HD13	1:11:A:PRO:HD2	10	0.43
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	7	0.42
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	7	0.42
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	7	0.42
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	7	0.42
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	7	0.42
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	7	0.42
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE1	6	0.42
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE2	6	0.42
(1,545)	1:34:A:THR:HG21	1:40:A:CYS:H	9	0.42
(1,545)	1:34:A:THR:HG22	1:40:A:CYS:H	9	0.42
(1,545)	1:34:A:THR:HG23	1:40:A:CYS:H	9	0.42
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB2	4	0.42
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB3	4	0.42
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB2	4	0.42
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB3	4	0.42
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB2	4	0.42
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB3	4	0.42
(1,209)	1:15:A:THR:HB	1:17:A:LYS:HE2	5	0.42
(1,209)	1:15:A:THR:HB	1:17:A:LYS:HE3	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	9	0.41
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	9	0.41
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	9	0.41
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	3	0.41
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	3	0.41
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	3	0.41
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	3	0.41
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	3	0.41
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	3	0.41
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	3	0.41
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	3	0.41
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	3	0.41
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	3	0.41
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	3	0.41
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	3	0.41
(1,1094)	1:65:A:GLN:HE21	1:80:A:LYS:HA	6	0.41
(1,1094)	1:65:A:GLN:HE22	1:80:A:LYS:HA	6	0.41
(1,1093)	1:65:A:GLN:HE21	1:80:A:LYS:HA	6	0.41
(1,1093)	1:65:A:GLN:HE22	1:80:A:LYS:HA	6	0.41
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	5	0.41
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	5	0.41
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	5	0.41
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	5	0.41
(1,351)	1:26:A:HIS:HD2	1:32:A:TRP:HE3	6	0.41
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	3	0.4
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	3	0.4
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	3	0.4
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	5	0.4
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	5	0.4
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	5	0.4
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	5	0.4
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	5	0.4
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	5	0.4
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	5	0.4
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	5	0.4
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	5	0.4
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	5	0.4
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	5	0.4
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	5	0.4
(1,151)	1:7:A:ASN:H	1:46:A:GLU:HB2	2	0.4
(1,151)	1:7:A:ASN:H	1:46:A:GLU:HB3	2	0.4
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	2	0.39
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	2	0.39
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	9	0.39
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	9	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	6	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	6	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	6	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	6	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	6	0.39
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	6	0.39
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	6	0.39
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD2	1	0.39
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD3	1	0.39
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD2	8	0.39
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD3	8	0.39
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	4	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	4	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	4	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	5	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	5	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	5	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	8	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	8	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	8	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	10	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	10	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	10	0.38
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	4	0.38
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	4	0.38
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	4	0.38
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	4	0.38
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	4	0.38
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	4	0.38
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB2	9	0.38
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB3	9	0.38
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB2	9	0.38
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB3	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	8	0.38
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	8	0.38
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	8	0.38
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	8	0.38
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	8	0.38
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	8	0.38
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	8	0.38
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	6	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	6	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	6	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	7	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	7	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	7	0.37
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	1	0.37
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	1	0.37
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	6	0.37
(1,288)	1:20:A:ASP:HB2	1:21:A:LEU:H	8	0.37
(1,288)	1:20:A:ASP:HB3	1:21:A:LEU:H	8	0.37
(1,287)	1:20:A:ASP:HB2	1:21:A:LEU:H	8	0.37
(1,287)	1:20:A:ASP:HB3	1:21:A:LEU:H	8	0.37
(1,256)	1:19:A:MET:HA	1:26:A:HIS:HD2	8	0.37
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD11	1	0.36
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD12	1	0.36
(1,1554)	1:94:A:ILE:HA	1:94:A:ILE:HD13	1	0.36
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	2	0.36
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	2	0.36
(1,265)	1:19:A:MET:HE1	1:25:A:LYS:HA	3	0.36
(1,265)	1:19:A:MET:HE2	1:25:A:LYS:HA	3	0.36
(1,265)	1:19:A:MET:HE3	1:25:A:LYS:HA	3	0.36
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	4	0.36
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	4	0.36
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	4	0.36
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	4	0.36
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	4	0.36
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	4	0.36
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	4	0.36
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	3	0.35
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	3	0.35
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	3	0.35
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	3	0.35
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	3	0.35
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	3	0.35
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	1	0.34
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	1	0.34
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	1	0.34
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	1	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	3	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	5	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	5	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	5	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	5	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	5	0.34
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	3	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	5	0.34
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	5	0.34
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD11	10	0.34
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD12	10	0.34
(1,1089)	1:65:A:GLN:HE21	1:67:A:ILE:HD13	10	0.34
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD11	10	0.34
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD12	10	0.34
(1,1089)	1:65:A:GLN:HE22	1:67:A:ILE:HD13	10	0.34
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	3	0.34
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	3	0.34
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	3	0.34
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	3	0.34
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	3	0.34
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	3	0.34
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB2	8	0.34
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB3	8	0.34
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB2	8	0.34
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB3	8	0.34
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG21	10	0.34
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG22	10	0.34
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG23	10	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG21	10	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG22	10	0.34
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG23	10	0.34
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD11	3	0.33
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD12	3	0.33
(1,1223)	1:69:A:LYS:HE2	1:76:A:ILE:HD13	3	0.33
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD11	3	0.33
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD12	3	0.33
(1,1223)	1:69:A:LYS:HE3	1:76:A:ILE:HD13	3	0.33
(1,558)	1:36:A:ASN:HB2	1:37:A:CYS:H	10	0.33
(1,558)	1:36:A:ASN:HB3	1:37:A:CYS:H	10	0.33
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	4	0.33
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	4	0.33
(1,525)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	4	0.33
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	4	0.33
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	4	0.33
(1,525)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	4	0.33
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD11	4	0.33
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD12	4	0.33
(1,524)	1:33:A:GLN:HE21	1:52:A:LEU:HD13	4	0.33
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD11	4	0.33
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD12	4	0.33
(1,524)	1:33:A:GLN:HE22	1:52:A:LEU:HD13	4	0.33
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	2	0.33
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	9	0.33
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	9	0.33
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	2	0.33
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	2	0.33
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	9	0.33
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	9	0.33
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	1	0.33
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	1	0.33
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	1	0.33
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	1	0.33
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD2	7	0.33
(1,208)	1:15:A:THR:HB	1:17:A:LYS:HD3	7	0.33
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB2	2	0.33
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB3	2	0.33
(1,139)	1:7:A:ASN:HB2	1:45:A:THR:HA	7	0.33
(1,139)	1:7:A:ASN:HB3	1:45:A:THR:HA	7	0.33
(1,138)	1:7:A:ASN:HB2	1:45:A:THR:HA	7	0.33
(1,138)	1:7:A:ASN:HB3	1:45:A:THR:HA	7	0.33
(1,1008)	1:60:A:ASP:HB2	1:63:A:ASN:H	10	0.32
(1,1008)	1:60:A:ASP:HB3	1:63:A:ASN:H	10	0.32
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	7	0.32
(1,720)	1:46:A:GLU:HB2	1:47:A:ILE:H	2	0.32
(1,720)	1:46:A:GLU:HB3	1:47:A:ILE:H	2	0.32
(1,719)	1:46:A:GLU:HB2	1:47:A:ILE:H	2	0.32
(1,719)	1:46:A:GLU:HB3	1:47:A:ILE:H	2	0.32
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	10	0.32
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	10	0.32
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	10	0.32
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	10	0.32
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	9	0.32
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	9	0.32
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	9	0.32
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	9	0.32
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	9	0.32
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	9	0.32
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	9	0.32
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	9	0.32
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	9	0.32
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	9	0.32
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	9	0.32
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	9	0.32
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE1	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE2	4	0.31
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE1	4	0.31
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE2	4	0.31
(1,813)	1:53:A:VAL:HG11	1:74:A:LYS:HA	6	0.31
(1,813)	1:53:A:VAL:HG12	1:74:A:LYS:HA	6	0.31
(1,813)	1:53:A:VAL:HG13	1:74:A:LYS:HA	6	0.31
(1,813)	1:53:A:VAL:HG21	1:74:A:LYS:HA	6	0.31
(1,813)	1:53:A:VAL:HG22	1:74:A:LYS:HA	6	0.31
(1,813)	1:53:A:VAL:HG23	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG11	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG12	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG13	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG21	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG22	1:74:A:LYS:HA	6	0.31
(1,812)	1:53:A:VAL:HG23	1:74:A:LYS:HA	6	0.31
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG2	8	0.31
(1,708)	1:44:A:GLU:H	1:44:A:GLU:HG3	8	0.31
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	3	0.31
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	3	0.31
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	3	0.31
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	3	0.31
(1,291)	1:20:A:ASP:HB2	1:32:A:TRP:HE1	8	0.31
(1,291)	1:20:A:ASP:HB3	1:32:A:TRP:HE1	8	0.31
(1,168)	1:8:A:GLU:H	1:8:A:GLU:HG2	5	0.31
(1,168)	1:8:A:GLU:H	1:8:A:GLU:HG3	5	0.31
(1,153)	1:7:A:ASN:H	1:47:A:ILE:H	6	0.31
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	9	0.3
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	9	0.3
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	9	0.3
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	9	0.3
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	10	0.3
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	9	0.3
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	9	0.3
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	9	0.3
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	9	0.3
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	5	0.3
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	5	0.3
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	5	0.3
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	5	0.3
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	5	0.3
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	5	0.3
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB2	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:27:A:PRO:HB2	1:30:A:SER:HB3	9	0.3
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB2	9	0.3
(1,361)	1:27:A:PRO:HB2	1:30:A:SER:HB3	9	0.3
(1,262)	1:19:A:MET:HE1	1:24:A:ASN:HA	3	0.3
(1,262)	1:19:A:MET:HE2	1:24:A:ASN:HA	3	0.3
(1,262)	1:19:A:MET:HE3	1:24:A:ASN:HA	3	0.3
(1,186)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	3	0.3
(1,186)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	3	0.3
(1,186)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	3	0.3
(1,186)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	3	0.3
(1,186)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	3	0.3
(1,186)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	3	0.3
(1,185)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	3	0.3
(1,1422)	1:81:A:LYS:HG2	1:82:A:ASP:H	2	0.29
(1,1422)	1:81:A:LYS:HG3	1:82:A:ASP:H	2	0.29
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	3	0.29
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	3	0.29
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	3	0.29
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	3	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG11	9	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG12	9	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG13	9	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG21	9	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG22	9	0.29
(1,1092)	1:65:A:GLN:HE21	1:78:A:VAL:HG23	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG11	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG12	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG13	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG21	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG22	9	0.29
(1,1092)	1:65:A:GLN:HE22	1:78:A:VAL:HG23	9	0.29
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	2	0.29
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	2	0.29
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	2	0.29
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	2	0.29
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	2	0.29
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	7	0.29
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	7	0.29
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	7	0.29
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	7	0.29
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	7	0.29
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	7	0.29
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	7	0.29
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	7	0.29
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	7	0.29
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	7	0.29
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	7	0.29
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	7	0.29
(1,558)	1:36:A:ASN:HB2	1:37:A:CYS:H	2	0.29
(1,558)	1:36:A:ASN:HB3	1:37:A:CYS:H	2	0.29
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	8	0.29
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	8	0.29
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	8	0.29
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	8	0.29
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD11	9	0.29
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD12	9	0.29
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD13	9	0.29
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	2	0.28
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	2	0.28
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	5	0.28
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	5	0.28
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	2	0.28
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	2	0.28
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	5	0.28
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	5	0.28
(1,940)	1:58:A:GLY:HA2	1:89:A:VAL:HG11	5	0.28
(1,940)	1:58:A:GLY:HA2	1:89:A:VAL:HG12	5	0.28
(1,940)	1:58:A:GLY:HA2	1:89:A:VAL:HG13	5	0.28
(1,940)	1:58:A:GLY:HA3	1:89:A:VAL:HG11	5	0.28
(1,940)	1:58:A:GLY:HA3	1:89:A:VAL:HG12	5	0.28
(1,940)	1:58:A:GLY:HA3	1:89:A:VAL:HG13	5	0.28
(1,199)	1:10:A:VAL:H	1:13:A:ASP:HB2	4	0.28
(1,199)	1:10:A:VAL:H	1:13:A:ASP:HB3	4	0.28
(1,169)	1:8:A:GLU:H	1:9:A:GLY:H	3	0.28
(1,135)	1:7:A:ASN:HA	1:47:A:ILE:HG13	10	0.28
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	8	0.27
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	8	0.27
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	8	0.27
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	8	0.27
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	8	0.27
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	8	0.27
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	8	0.27
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	8	0.27
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	8	0.27
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	8	0.27
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	8	0.27
(1,1373)	1:78:A:VAL:HG11	1:79:A:GLU:H	7	0.27
(1,1373)	1:78:A:VAL:HG12	1:79:A:GLU:H	7	0.27
(1,1373)	1:78:A:VAL:HG13	1:79:A:GLU:H	7	0.27
(1,1373)	1:78:A:VAL:HG21	1:79:A:GLU:H	7	0.27
(1,1373)	1:78:A:VAL:HG22	1:79:A:GLU:H	7	0.27
(1,1373)	1:78:A:VAL:HG23	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG11	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG12	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG13	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG21	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG22	1:79:A:GLU:H	7	0.27
(1,1372)	1:78:A:VAL:HG23	1:79:A:GLU:H	7	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	4	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	4	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	8	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	8	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB2	10	0.27
(1,1067)	1:64:A:CYS:HB3	1:87:A:CYS:HB3	10	0.27
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG11	5	0.27
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG12	5	0.27
(1,959)	1:59:A:TYR:HB2	1:89:A:VAL:HG13	5	0.27
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG11	5	0.27
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG12	5	0.27
(1,959)	1:59:A:TYR:HB3	1:89:A:VAL:HG13	5	0.27
(1,891)	1:56:A:PRO:HA	1:92:A:TRP:HE3	8	0.27
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	7	0.27
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	7	0.27
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	7	0.27
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	7	0.27
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	7	0.27
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	7	0.27
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	7	0.27
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	7	0.27
(1,290)	1:20:A:ASP:HB2	1:32:A:TRP:HD1	9	0.27
(1,290)	1:20:A:ASP:HB3	1:32:A:TRP:HD1	9	0.27
(1,256)	1:19:A:MET:HA	1:26:A:HIS:HD2	3	0.27
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE2	3	0.27
(1,228)	1:17:A:LYS:HB2	1:17:A:LYS:HE3	3	0.27
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE2	3	0.27
(1,228)	1:17:A:LYS:HB3	1:17:A:LYS:HE3	3	0.27
(1,203)	1:12:A:GLY:H	1:13:A:ASP:H	4	0.27
(1,153)	1:7:A:ASN:H	1:47:A:ILE:H	2	0.27
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	1	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	1	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	1	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	1	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	1	0.26
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	1	0.26
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	1	0.26
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	1	0.26
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	1	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	1	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	1	0.26
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	1	0.26
(1,1471)	1:87:A:CYS:HB2	1:88:A:SER:H	3	0.26
(1,1471)	1:87:A:CYS:HB3	1:88:A:SER:H	3	0.26
(1,1470)	1:87:A:CYS:HB2	1:88:A:SER:H	3	0.26
(1,1470)	1:87:A:CYS:HB3	1:88:A:SER:H	3	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG11	9	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG12	9	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG13	9	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG21	9	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG22	9	0.26
(1,1132)	1:66:A:ARG:HG2	1:77:A:VAL:HG23	9	0.26
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG11	9	0.26
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG12	9	0.26
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG13	9	0.26
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG21	9	0.26
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG22	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:66:A:ARG:HG3	1:77:A:VAL:HG23	9	0.26
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE1	2	0.26
(1,1131)	1:66:A:ARG:HG2	1:75:A:TYR:HE2	2	0.26
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE1	2	0.26
(1,1131)	1:66:A:ARG:HG3	1:75:A:TYR:HE2	2	0.26
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	1	0.26
(1,784)	1:52:A:LEU:H	1:53:A:VAL:H	9	0.26
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB2	9	0.26
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB3	9	0.26
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB2	9	0.26
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB3	9	0.26
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	4	0.26
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	4	0.26
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	4	0.26
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	4	0.26
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	5	0.26
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	5	0.26
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	5	0.26
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	5	0.26
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	5	0.26
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	5	0.26
(1,194)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	5	0.26
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	5	0.26
(1,193)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	5	0.26
(1,192)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	5	0.26
(1,192)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	5	0.26
(1,192)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	5	0.26
(1,192)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	5	0.26
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	5	0.26
(1,192)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG11	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG12	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG13	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG21	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG22	1:13:A:ASP:HB3	5	0.26
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB2	5	0.26
(1,191)	1:10:A:VAL:HG23	1:13:A:ASP:HB3	5	0.26
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	4	0.25
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	4	0.25
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	4	0.25
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	4	0.25
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	4	0.25
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	4	0.25
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	4	0.25
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	4	0.25
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	4	0.25
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	4	0.25
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	4	0.25
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	4	0.25
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	5	0.25
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	5	0.25
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	5	0.25
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	5	0.25
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	8	0.25
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	8	0.25
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	8	0.25
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	8	0.25
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	8	0.25
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	8	0.25
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	8	0.25
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	8	0.25
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	8	0.25
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	8	0.25
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	8	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	5	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	5	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	5	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	5	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	5	0.25
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	5	0.25
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	5	0.25
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB2	2	0.25
(1,266)	1:19:A:MET:HE1	1:25:A:LYS:HB3	2	0.25
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB2	2	0.25
(1,266)	1:19:A:MET:HE2	1:25:A:LYS:HB3	2	0.25
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB2	2	0.25
(1,266)	1:19:A:MET:HE3	1:25:A:LYS:HB3	2	0.25
(1,143)	1:7:A:ASN:HB2	1:46:A:GLU:H	9	0.25
(1,143)	1:7:A:ASN:HB3	1:46:A:GLU:H	9	0.25
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	10	0.24
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	10	0.24
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	10	0.24
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	10	0.24
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	10	0.24
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	10	0.24
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	10	0.24
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	10	0.24
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	10	0.24
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	10	0.24
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	10	0.24
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	10	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	4	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	4	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	8	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	10	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	10	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	4	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	4	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	8	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	8	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	10	0.24
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	10	0.24
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	3	0.24
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	3	0.24
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	3	0.24
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	3	0.24
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	6	0.24
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	6	0.24
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	6	0.24
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	6	0.24
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB2	7	0.23
(1,1330)	1:77:A:VAL:HB	1:87:A:CYS:HB3	7	0.23
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB2	7	0.23
(1,1329)	1:77:A:VAL:HB	1:87:A:CYS:HB3	7	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	2	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	2	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	2	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	2	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	7	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	7	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	7	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	7	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	8	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	8	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	8	0.23
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	8	0.23
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE1	1	0.23
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE2	1	0.23
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE1	5	0.23
(1,798)	1:53:A:VAL:HB	1:75:A:TYR:HE2	5	0.23
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB2	8	0.23
(1,544)	1:34:A:THR:HG21	1:40:A:CYS:HB3	8	0.23
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB2	8	0.23
(1,544)	1:34:A:THR:HG22	1:40:A:CYS:HB3	8	0.23
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB2	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:34:A:THR:HG23	1:40:A:CYS:HB3	8	0.23
(1,276)	1:19:A:MET:HG2	1:25:A:LYS:HA	2	0.23
(1,276)	1:19:A:MET:HG3	1:25:A:LYS:HA	2	0.23
(1,259)	1:19:A:MET:HE1	1:23:A:GLY:HA2	2	0.23
(1,259)	1:19:A:MET:HE2	1:23:A:GLY:HA2	2	0.23
(1,259)	1:19:A:MET:HE3	1:23:A:GLY:HA2	2	0.23
(1,195)	1:10:A:VAL:HG11	1:13:A:ASP:H	10	0.23
(1,195)	1:10:A:VAL:HG12	1:13:A:ASP:H	10	0.23
(1,195)	1:10:A:VAL:HG13	1:13:A:ASP:H	10	0.23
(1,195)	1:10:A:VAL:HG21	1:13:A:ASP:H	10	0.23
(1,195)	1:10:A:VAL:HG22	1:13:A:ASP:H	10	0.23
(1,195)	1:10:A:VAL:HG23	1:13:A:ASP:H	10	0.23
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	9	0.22
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	9	0.22
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	9	0.22
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	9	0.22
(1,1009)	1:60:A:ASP:HB2	1:64:A:CYS:H	2	0.22
(1,1009)	1:60:A:ASP:HB3	1:64:A:CYS:H	2	0.22
(1,1009)	1:60:A:ASP:HB2	1:64:A:CYS:H	4	0.22
(1,1009)	1:60:A:ASP:HB3	1:64:A:CYS:H	4	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	9	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	9	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	9	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	9	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	9	0.22
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	9	0.22
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	9	0.22
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	9	0.22
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	9	0.22
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	9	0.22
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	9	0.22
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	9	0.22
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	9	0.22
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB2	7	0.22
(1,975)	1:59:A:TYR:HD1	1:87:A:CYS:HB3	7	0.22
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB2	7	0.22
(1,975)	1:59:A:TYR:HD2	1:87:A:CYS:HB3	7	0.22
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	5	0.22
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	5	0.22
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	5	0.22
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	5	0.22
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	5	0.22
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	5	0.22
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	5	0.22
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	5	0.22
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	5	0.22
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	5	0.22
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	5	0.22
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	5	0.22
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	5	0.22
(1,876)	1:55:A:THR:H	1:93:A:ILE:HB	6	0.22
(1,560)	1:36:A:ASN:HB2	1:37:A:CYS:H	3	0.22
(1,560)	1:36:A:ASN:HB3	1:37:A:CYS:H	3	0.22
(1,559)	1:36:A:ASN:HB2	1:37:A:CYS:H	3	0.22
(1,559)	1:36:A:ASN:HB3	1:37:A:CYS:H	3	0.22
(1,545)	1:34:A:THR:HG21	1:40:A:CYS:H	7	0.22
(1,545)	1:34:A:THR:HG22	1:40:A:CYS:H	7	0.22
(1,545)	1:34:A:THR:HG23	1:40:A:CYS:H	7	0.22
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	8	0.22
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	8	0.22
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	8	0.22
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	8	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	2	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	2	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	2	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	2	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	2	0.22
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	2	0.22
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	2	0.22
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	2	0.22
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	2	0.22
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	2	0.22
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	2	0.22
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD11	2	0.22
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD12	2	0.22
(1,134)	1:7:A:ASN:HA	1:47:A:ILE:HD13	2	0.22
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	7	0.22
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	7	0.22
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	7	0.22
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	7	0.22
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	7	0.22
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	7	0.22
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	7	0.22
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	7	0.22
(1,1009)	1:60:A:ASP:HB2	1:64:A:CYS:H	6	0.21
(1,1009)	1:60:A:ASP:HB3	1:64:A:CYS:H	6	0.21
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	1	0.21
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	1	0.21
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	1	0.21
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	1	0.21
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	1	0.21
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	1	0.21
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	1	0.21
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	1	0.21
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	1	0.21
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	1	0.21
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	1	0.21
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	1	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	9	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	9	0.21
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	9	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	9	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	9	0.21
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	9	0.21
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	9	0.21
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	9	0.21
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	9	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	9	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	9	0.21
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	9	0.21
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	1	0.21
(1,498)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	1	0.21
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB2	1	0.21
(1,497)	1:32:A:TRP:HZ2	1:40:A:CYS:HB3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	5	0.21
(1,481)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	5	0.21
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	5	0.21
(1,480)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	5	0.21
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD11	3	0.21
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD12	3	0.21
(1,249)	1:18:A:CYS:H	1:47:A:ILE:HD13	3	0.21
(1,145)	1:7:A:ASN:HB2	1:47:A:ILE:HG13	2	0.21
(1,145)	1:7:A:ASN:HB3	1:47:A:ILE:HG13	2	0.21
(1,1307)	1:75:A:TYR:H	1:92:A:TRP:HZ3	4	0.2
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG2	9	0.2
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG3	9	0.2
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG2	10	0.2
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG3	10	0.2
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE2	3	0.2
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE3	3	0.2
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	6	0.2
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	6	0.2
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	6	0.2
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	6	0.2
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	6	0.2
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	6	0.2
(1,837)	1:54:A:SER:HB2	1:94:A:ILE:HB	2	0.2
(1,837)	1:54:A:SER:HB3	1:94:A:ILE:HB	2	0.2
(1,836)	1:54:A:SER:HB2	1:94:A:ILE:HB	2	0.2
(1,836)	1:54:A:SER:HB3	1:94:A:ILE:HB	2	0.2
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	3	0.2
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	3	0.2
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	3	0.2
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	3	0.2
(1,527)	1:33:A:GLN:HG2	1:34:A:THR:H	4	0.2
(1,527)	1:33:A:GLN:HG3	1:34:A:THR:H	4	0.2
(1,526)	1:33:A:GLN:HG2	1:34:A:THR:H	4	0.2
(1,526)	1:33:A:GLN:HG3	1:34:A:THR:H	4	0.2
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG21	1	0.2
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG22	1	0.2
(1,116)	1:5:A:ILE:H	1:47:A:ILE:HG23	1	0.2
(1,1356)	1:77:A:VAL:HG11	1:92:A:TRP:HZ2	2	0.19
(1,1356)	1:77:A:VAL:HG12	1:92:A:TRP:HZ2	2	0.19
(1,1356)	1:77:A:VAL:HG13	1:92:A:TRP:HZ2	2	0.19
(1,1356)	1:77:A:VAL:HG21	1:92:A:TRP:HZ2	2	0.19
(1,1356)	1:77:A:VAL:HG22	1:92:A:TRP:HZ2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1356)	1:77:A:VAL:HG23	1:92:A:TRP:HZ2	2	0.19
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG2	8	0.19
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG3	8	0.19
(1,1094)	1:65:A:GLN:HE21	1:80:A:LYS:HA	7	0.19
(1,1094)	1:65:A:GLN:HE22	1:80:A:LYS:HA	7	0.19
(1,1093)	1:65:A:GLN:HE21	1:80:A:LYS:HA	7	0.19
(1,1093)	1:65:A:GLN:HE22	1:80:A:LYS:HA	7	0.19
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	6	0.19
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	6	0.19
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	6	0.19
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	6	0.19
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	6	0.19
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	6	0.19
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	9	0.19
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	9	0.19
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	9	0.19
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	9	0.19
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	9	0.19
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	9	0.19
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	6	0.19
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	6	0.19
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	6	0.19
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	6	0.19
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	6	0.19
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	6	0.19
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	9	0.19
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	9	0.19
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	9	0.19
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	9	0.19
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	9	0.19
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	9	0.19
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	8	0.19
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	8	0.19
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	8	0.19
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	8	0.19
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	8	0.19
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	8	0.19
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG2	5	0.19
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG3	5	0.19
(1,265)	1:19:A:MET:HE1	1:25:A:LYS:HA	8	0.19
(1,265)	1:19:A:MET:HE2	1:25:A:LYS:HA	8	0.19
(1,265)	1:19:A:MET:HE3	1:25:A:LYS:HA	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD2	2	0.19
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD3	2	0.19
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG21	8	0.19
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG22	8	0.19
(1,206)	1:14:A:SER:HB2	1:15:A:THR:HG23	8	0.19
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG21	8	0.19
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG22	8	0.19
(1,206)	1:14:A:SER:HB3	1:15:A:THR:HG23	8	0.19
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	4	0.19
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	4	0.19
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	4	0.19
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	4	0.19
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	4	0.19
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	4	0.19
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	4	0.19
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	4	0.19
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	4	0.19
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	4	0.19
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	4	0.19
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	4	0.19
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	5	0.19
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	5	0.19
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	5	0.19
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	5	0.19
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	5	0.19
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	5	0.19
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	5	0.19
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	5	0.19
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	1	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	1	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	1	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	1	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	1	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	1	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	2	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	2	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	2	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	2	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	2	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	2	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	3	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	3	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	3	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	3	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	3	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	4	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	4	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	4	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	4	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	4	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	4	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	5	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	5	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	5	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	5	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	5	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	5	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	7	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	7	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	7	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	7	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	7	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	7	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	9	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	9	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	9	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	9	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	9	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	9	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	10	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	10	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	10	0.18
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	10	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	10	0.18
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	10	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	1	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	1	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	1	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	1	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	1	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	1	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	2	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	2	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	2	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	2	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	2	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	3	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	3	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	3	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	3	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	3	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	3	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	4	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	4	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	4	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	4	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	4	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	4	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	5	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	5	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	5	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	5	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	5	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	5	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	7	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	7	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	7	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	7	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	7	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	7	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	9	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	9	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	9	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	9	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	9	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	9	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	10	0.18
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	10	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	10	0.18
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	10	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	10	0.18
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	10	0.18
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG2	2	0.18
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG2	2	0.18
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG3	2	0.18
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG2	7	0.18
(1,1201)	1:68:A:PHE:HZ	1:70:A:LYS:HG3	7	0.18
(1,1009)	1:60:A:ASP:HB2	1:64:A:CYS:H	8	0.18
(1,1009)	1:60:A:ASP:HB3	1:64:A:CYS:H	8	0.18
(1,527)	1:33:A:GLN:HG2	1:34:A:THR:H	9	0.18
(1,527)	1:33:A:GLN:HG3	1:34:A:THR:H	9	0.18
(1,526)	1:33:A:GLN:HG2	1:34:A:THR:H	9	0.18
(1,526)	1:33:A:GLN:HG3	1:34:A:THR:H	9	0.18
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB2	10	0.18
(1,479)	1:32:A:TRP:HE1	1:40:A:CYS:HB3	10	0.18
(1,291)	1:20:A:ASP:HB2	1:32:A:TRP:HE1	3	0.18
(1,291)	1:20:A:ASP:HB3	1:32:A:TRP:HE1	3	0.18
(1,262)	1:19:A:MET:HE1	1:24:A:ASN:HA	9	0.18
(1,262)	1:19:A:MET:HE2	1:24:A:ASN:HA	9	0.18
(1,262)	1:19:A:MET:HE3	1:24:A:ASN:HA	9	0.18
(1,186)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	5	0.18
(1,186)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	5	0.18
(1,186)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	5	0.18
(1,186)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	5	0.18
(1,186)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	5	0.18
(1,186)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	5	0.18
(1,185)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	5	0.18
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	3	0.18
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	3	0.18
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	3	0.18
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	3	0.18
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	3	0.18
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	3	0.18
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	3	0.18
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	3	0.18
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	6	0.17
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	6	0.17
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	6	0.17
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	6	0.17
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	6	0.17
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	8	0.17
(1,1560)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	8	0.17
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	8	0.17
(1,1560)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	8	0.17
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	8	0.17
(1,1560)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	8	0.17
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	6	0.17
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	6	0.17
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	6	0.17
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	6	0.17
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	6	0.17
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	6	0.17
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG12	8	0.17
(1,1559)	1:94:A:ILE:HG21	1:94:A:ILE:HG13	8	0.17
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG12	8	0.17
(1,1559)	1:94:A:ILE:HG22	1:94:A:ILE:HG13	8	0.17
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG12	8	0.17
(1,1559)	1:94:A:ILE:HG23	1:94:A:ILE:HG13	8	0.17
(1,1471)	1:87:A:CYS:HB2	1:88:A:SER:H	5	0.17
(1,1471)	1:87:A:CYS:HB3	1:88:A:SER:H	5	0.17
(1,1470)	1:87:A:CYS:HB2	1:88:A:SER:H	5	0.17
(1,1470)	1:87:A:CYS:HB3	1:88:A:SER:H	5	0.17
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG2	1	0.17
(1,1191)	1:68:A:PHE:HE1	1:70:A:LYS:HG3	1	0.17
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG2	1	0.17
(1,1191)	1:68:A:PHE:HE2	1:70:A:LYS:HG3	1	0.17
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	9	0.17
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	9	0.17
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	9	0.17
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	9	0.17
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	9	0.17
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	9	0.17
(1,35)	1:3:A:TYR:HD1	1:4:A:PHE:HA	8	0.17
(1,35)	1:3:A:TYR:HD2	1:4:A:PHE:HA	8	0.17
(1,1518)	1:91:A:GLU:HA	1:92:A:TRP:HD1	8	0.16
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	2	0.16
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	2	0.16
(1,1474)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	2	0.16
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	2	0.16
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	2	0.16
(1,1474)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG21	2	0.16
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG22	2	0.16
(1,1473)	1:87:A:CYS:HB2	1:89:A:VAL:HG23	2	0.16
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG21	2	0.16
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG22	2	0.16
(1,1473)	1:87:A:CYS:HB3	1:89:A:VAL:HG23	2	0.16
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	1	0.16
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	1	0.16
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	6	0.16
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	6	0.16
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	1	0.16
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	1	0.16
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	6	0.16
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	6	0.16
(1,1189)	1:68:A:PHE:HE1	1:70:A:LYS:HB2	4	0.16
(1,1189)	1:68:A:PHE:HE1	1:70:A:LYS:HB3	4	0.16
(1,1189)	1:68:A:PHE:HE2	1:70:A:LYS:HB2	4	0.16
(1,1189)	1:68:A:PHE:HE2	1:70:A:LYS:HB3	4	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	7	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	7	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	7	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	7	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	7	0.16
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	7	0.16
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	7	0.16
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE2	5	0.16
(1,1074)	1:64:A:CYS:H	1:80:A:LYS:HE3	5	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	7	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	7	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	7	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	7	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	7	0.16
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	7	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	7	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	7	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	7	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	7	0.16
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	7	0.16
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	7	0.16
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	7	0.16
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	2	0.16
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	2	0.16
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	2	0.16
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	2	0.16
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	2	0.16
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	2	0.16
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	9	0.16
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB2	2	0.16
(1,621)	1:40:A:CYS:HA	1:49:A:CYS:HB3	2	0.16
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB2	2	0.16
(1,620)	1:40:A:CYS:HA	1:49:A:CYS:HB3	2	0.16
(1,562)	1:36:A:ASN:H	1:37:A:CYS:H	8	0.16
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG2	2	0.16
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG3	2	0.16
(1,351)	1:26:A:HIS:HD2	1:32:A:TRP:HE3	2	0.16
(1,288)	1:20:A:ASP:HB2	1:21:A:LEU:H	5	0.16
(1,288)	1:20:A:ASP:HB3	1:21:A:LEU:H	5	0.16
(1,287)	1:20:A:ASP:HB2	1:21:A:LEU:H	5	0.16
(1,287)	1:20:A:ASP:HB3	1:21:A:LEU:H	5	0.16
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB2	6	0.16
(1,181)	1:10:A:VAL:HB	1:13:A:ASP:HB3	6	0.16
(1,153)	1:7:A:ASN:H	1:47:A:ILE:H	5	0.16
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	6	0.16
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	6	0.16
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	6	0.16
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	6	0.16
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	6	0.16
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	6	0.16
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	6	0.16
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	6	0.16
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	6	0.16
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	6	0.16
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	6	0.16
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	8	0.15
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	8	0.15
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	8	0.15
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	8	0.15
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG2	8	0.15
(1,1251)	1:71:A:GLU:H	1:71:A:GLU:HG3	8	0.15
(1,1171)	1:68:A:PHE:HA	1:75:A:TYR:HE1	4	0.15
(1,1171)	1:68:A:PHE:HA	1:75:A:TYR:HE2	4	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG11	2	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG12	2	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG13	2	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG21	2	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG22	2	0.15
(1,1084)	1:65:A:GLN:HA	1:77:A:VAL:HG23	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG11	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG12	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG13	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG21	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG22	2	0.15
(1,1083)	1:65:A:GLN:HA	1:77:A:VAL:HG23	2	0.15
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	10	0.15
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	10	0.15
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	10	0.15
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	10	0.15
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	10	0.15
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	10	0.15
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	10	0.15
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	10	0.15
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	10	0.15
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	10	0.15
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	10	0.15
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	10	0.15
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD1	5	0.15
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD2	5	0.15
(1,709)	1:44:A:GLU:H	1:45:A:THR:HG21	2	0.15
(1,709)	1:44:A:GLU:H	1:45:A:THR:HG22	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,709)	1:44:A:GLU:H	1:45:A:THR:HG23	2	0.15
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG21	5	0.15
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG22	5	0.15
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG23	5	0.15
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG21	5	0.15
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG22	5	0.15
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG23	5	0.15
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG21	5	0.15
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG22	5	0.15
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG23	5	0.15
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG21	5	0.15
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG22	5	0.15
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG23	5	0.15
(1,319)	1:22:A:LYS:HB2	1:24:A:ASN:H	8	0.15
(1,319)	1:22:A:LYS:HB3	1:24:A:ASN:H	8	0.15
(1,318)	1:22:A:LYS:HB2	1:24:A:ASN:H	8	0.15
(1,318)	1:22:A:LYS:HB3	1:24:A:ASN:H	8	0.15
(1,186)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	6	0.15
(1,186)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	6	0.15
(1,186)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	6	0.15
(1,186)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	6	0.15
(1,186)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	6	0.15
(1,186)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	6	0.15
(1,185)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	6	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	6	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	6	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	6	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	6	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	8	0.15
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	8	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	8	0.15
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	8	0.15
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	6	0.15
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	6	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	6	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	6	0.15
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	8	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	8	0.15
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	8	0.15
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	7	0.14
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	7	0.14
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	7	0.14
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	7	0.14
(1,1180)	1:68:A:PHE:HD1	1:70:A:LYS:HG2	5	0.14
(1,1180)	1:68:A:PHE:HD1	1:70:A:LYS:HG3	5	0.14
(1,1180)	1:68:A:PHE:HD2	1:70:A:LYS:HG2	5	0.14
(1,1180)	1:68:A:PHE:HD2	1:70:A:LYS:HG3	5	0.14
(1,595)	1:38:A:GLU:H	1:52:A:LEU:HD11	5	0.14
(1,595)	1:38:A:GLU:H	1:52:A:LEU:HD12	5	0.14
(1,595)	1:38:A:GLU:H	1:52:A:LEU:HD13	5	0.14
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD11	7	0.14
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD12	7	0.14
(1,585)	1:38:A:GLU:HA	1:52:A:LEU:HD13	7	0.14
(1,410)	1:28:A:ILE:HG21	1:29:A:ASN:HD21	4	0.14
(1,410)	1:28:A:ILE:HG21	1:29:A:ASN:HD22	4	0.14
(1,410)	1:28:A:ILE:HG22	1:29:A:ASN:HD21	4	0.14
(1,410)	1:28:A:ILE:HG22	1:29:A:ASN:HD22	4	0.14
(1,410)	1:28:A:ILE:HG23	1:29:A:ASN:HD21	4	0.14
(1,410)	1:28:A:ILE:HG23	1:29:A:ASN:HD22	4	0.14
(1,409)	1:28:A:ILE:HG21	1:29:A:ASN:HD21	4	0.14
(1,409)	1:28:A:ILE:HG21	1:29:A:ASN:HD22	4	0.14
(1,409)	1:28:A:ILE:HG22	1:29:A:ASN:HD21	4	0.14
(1,409)	1:28:A:ILE:HG22	1:29:A:ASN:HD22	4	0.14
(1,409)	1:28:A:ILE:HG23	1:29:A:ASN:HD21	4	0.14
(1,409)	1:28:A:ILE:HG23	1:29:A:ASN:HD22	4	0.14
(1,288)	1:20:A:ASP:HB2	1:21:A:LEU:H	9	0.14
(1,288)	1:20:A:ASP:HB3	1:21:A:LEU:H	9	0.14
(1,287)	1:20:A:ASP:HB2	1:21:A:LEU:H	9	0.14
(1,287)	1:20:A:ASP:HB3	1:21:A:LEU:H	9	0.14
(1,262)	1:19:A:MET:HE1	1:24:A:ASN:HA	8	0.14
(1,262)	1:19:A:MET:HE2	1:24:A:ASN:HA	8	0.14
(1,262)	1:19:A:MET:HE3	1:24:A:ASN:HA	8	0.14
(1,224)	1:16:A:ARG:H	1:17:A:LYS:H	5	0.14
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	8	0.14
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	8	0.14
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	8	0.14
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	8	0.14
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	8	0.14
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	8	0.14
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	8	0.14
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG12	3	0.13
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG13	3	0.13
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG12	3	0.13
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG13	3	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	6	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	6	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	6	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	6	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	6	0.13
(1,993)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	6	0.13
(1,993)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG11	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG12	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG13	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG21	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG22	6	0.13
(1,992)	1:59:A:TYR:HE1	1:77:A:VAL:HG23	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG11	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG12	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG13	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG21	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG22	6	0.13
(1,992)	1:59:A:TYR:HE2	1:77:A:VAL:HG23	6	0.13
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	4	0.13
(1,931)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	4	0.13
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	4	0.13
(1,931)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	4	0.13
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	4	0.13
(1,931)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	4	0.13
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG12	4	0.13
(1,930)	1:57:A:VAL:HG11	1:93:A:ILE:HG13	4	0.13
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG12	4	0.13
(1,930)	1:57:A:VAL:HG12	1:93:A:ILE:HG13	4	0.13
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:57:A:VAL:HG13	1:93:A:ILE:HG13	4	0.13
(1,892)	1:56:A:PRO:HA	1:92:A:TRP:HZ3	3	0.13
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD1	2	0.13
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD2	2	0.13
(1,793)	1:53:A:VAL:HB	1:54:A:SER:H	9	0.13
(1,677)	1:43:A:TYR:HB3	1:46:A:GLU:HB2	1	0.13
(1,677)	1:43:A:TYR:HB3	1:46:A:GLU:HB3	1	0.13
(1,590)	1:38:A:GLU:HB2	1:51:A:THR:HA	8	0.13
(1,590)	1:38:A:GLU:HB3	1:51:A:THR:HA	8	0.13
(1,589)	1:38:A:GLU:HB2	1:51:A:THR:HA	8	0.13
(1,589)	1:38:A:GLU:HB3	1:51:A:THR:HA	8	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD11	3	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD12	3	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD13	3	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD21	3	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD22	3	0.13
(1,296)	1:21:A:LEU:HA	1:21:A:LEU:HD23	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD11	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD12	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD13	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD21	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD22	3	0.13
(1,295)	1:21:A:LEU:HA	1:21:A:LEU:HD23	3	0.13
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD2	5	0.13
(1,215)	1:16:A:ARG:HA	1:16:A:ARG:HD3	5	0.13
(1,203)	1:12:A:GLY:H	1:13:A:ASP:H	5	0.13
(1,186)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	9	0.13
(1,186)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	9	0.13
(1,186)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	9	0.13
(1,186)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	9	0.13
(1,186)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	9	0.13
(1,186)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG11	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG12	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG13	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG21	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG22	1:11:A:PRO:HD2	9	0.13
(1,185)	1:10:A:VAL:HG23	1:11:A:PRO:HD2	9	0.13
(1,145)	1:7:A:ASN:HB2	1:47:A:ILE:HG13	6	0.13
(1,145)	1:7:A:ASN:HB3	1:47:A:ILE:HG13	6	0.13
(1,139)	1:7:A:ASN:HB2	1:45:A:THR:HA	3	0.13
(1,139)	1:7:A:ASN:HB3	1:45:A:THR:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:7:A:ASN:HB2	1:45:A:THR:HA	3	0.13
(1,138)	1:7:A:ASN:HB3	1:45:A:THR:HA	3	0.13
(1,130)	1:6:A:PRO:HB2	1:9:A:GLY:H	10	0.13
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB2	3	0.13
(1,122)	1:6:A:PRO:HA	1:46:A:GLU:HB3	3	0.13
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	9	0.13
(1,112)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	9	0.13
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	9	0.13
(1,112)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	9	0.13
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	9	0.13
(1,112)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	9	0.13
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD2	9	0.13
(1,111)	1:5:A:ILE:HG21	1:6:A:PRO:HD3	9	0.13
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD2	9	0.13
(1,111)	1:5:A:ILE:HG22	1:6:A:PRO:HD3	9	0.13
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD2	9	0.13
(1,111)	1:5:A:ILE:HG23	1:6:A:PRO:HD3	9	0.13
(1,35)	1:3:A:TYR:HD1	1:4:A:PHE:HA	3	0.13
(1,35)	1:3:A:TYR:HD2	1:4:A:PHE:HA	3	0.13
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG2	4	0.12
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG3	4	0.12
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG2	4	0.12
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG3	4	0.12
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG12	8	0.12
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG13	8	0.12
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG12	8	0.12
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG13	8	0.12
(1,1262)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	3	0.12
(1,1262)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	3	0.12
(1,1261)	1:72:A:ASP:HB2	1:74:A:LYS:HG2	3	0.12
(1,1261)	1:72:A:ASP:HB3	1:74:A:LYS:HG2	3	0.12
(1,1088)	1:65:A:GLN:HB2	1:80:A:LYS:HE2	9	0.12
(1,1088)	1:65:A:GLN:HB2	1:80:A:LYS:HE3	9	0.12
(1,1088)	1:65:A:GLN:HB3	1:80:A:LYS:HE2	9	0.12
(1,1088)	1:65:A:GLN:HB3	1:80:A:LYS:HE3	9	0.12
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	3	0.12
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	3	0.12
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	3	0.12
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	3	0.12
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	3	0.12
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	3	0.12
(1,914)	1:57:A:VAL:H	1:59:A:TYR:HD1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:57:A:VAL:H	1:59:A:TYR:HD2	8	0.12
(1,844)	1:54:A:SER:HB2	1:94:A:ILE:HG21	9	0.12
(1,844)	1:54:A:SER:HB2	1:94:A:ILE:HG22	9	0.12
(1,844)	1:54:A:SER:HB2	1:94:A:ILE:HG23	9	0.12
(1,844)	1:54:A:SER:HB3	1:94:A:ILE:HG21	9	0.12
(1,844)	1:54:A:SER:HB3	1:94:A:ILE:HG22	9	0.12
(1,844)	1:54:A:SER:HB3	1:94:A:ILE:HG23	9	0.12
(1,843)	1:54:A:SER:HB2	1:94:A:ILE:HG21	9	0.12
(1,843)	1:54:A:SER:HB2	1:94:A:ILE:HG22	9	0.12
(1,843)	1:54:A:SER:HB2	1:94:A:ILE:HG23	9	0.12
(1,843)	1:54:A:SER:HB3	1:94:A:ILE:HG21	9	0.12
(1,843)	1:54:A:SER:HB3	1:94:A:ILE:HG22	9	0.12
(1,843)	1:54:A:SER:HB3	1:94:A:ILE:HG23	9	0.12
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD1	3	0.12
(1,797)	1:53:A:VAL:HB	1:75:A:TYR:HD2	3	0.12
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG21	3	0.12
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG22	3	0.12
(1,705)	1:44:A:GLU:HB2	1:45:A:THR:HG23	3	0.12
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG21	3	0.12
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG22	3	0.12
(1,705)	1:44:A:GLU:HB3	1:45:A:THR:HG23	3	0.12
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG21	3	0.12
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG22	3	0.12
(1,704)	1:44:A:GLU:HB2	1:45:A:THR:HG23	3	0.12
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG21	3	0.12
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG22	3	0.12
(1,704)	1:44:A:GLU:HB3	1:45:A:THR:HG23	3	0.12
(1,517)	1:33:A:GLN:HA	1:39:A:THR:HG21	9	0.12
(1,517)	1:33:A:GLN:HA	1:39:A:THR:HG22	9	0.12
(1,517)	1:33:A:GLN:HA	1:39:A:THR:HG23	9	0.12
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG2	3	0.12
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG3	3	0.12
(1,431)	1:30:A:SER:HA	1:31:A:GLU:HG2	9	0.12
(1,431)	1:30:A:SER:HA	1:31:A:GLU:HG3	9	0.12
(1,323)	1:22:A:LYS:H	1:22:A:LYS:HD2	9	0.12
(1,323)	1:22:A:LYS:H	1:22:A:LYS:HD3	9	0.12
(1,319)	1:22:A:LYS:HB2	1:24:A:ASN:H	3	0.12
(1,319)	1:22:A:LYS:HB3	1:24:A:ASN:H	3	0.12
(1,318)	1:22:A:LYS:HB2	1:24:A:ASN:H	3	0.12
(1,318)	1:22:A:LYS:HB3	1:24:A:ASN:H	3	0.12
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	5	0.12
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	5	0.12
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	5	0.12
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	6	0.12
(1,41)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	6	0.12
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	6	0.12
(1,41)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	6	0.12
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	5	0.12
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	5	0.12
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	5	0.12
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	5	0.12
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG12	6	0.12
(1,40)	1:3:A:TYR:HD1	1:5:A:ILE:HG13	6	0.12
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG12	6	0.12
(1,40)	1:3:A:TYR:HD2	1:5:A:ILE:HG13	6	0.12
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG2	2	0.11
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG3	2	0.11
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG2	10	0.11
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG3	10	0.11
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG2	2	0.11
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG3	2	0.11
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG2	10	0.11
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG3	10	0.11
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG12	4	0.11
(1,1296)	1:75:A:TYR:HA	1:76:A:ILE:HG13	4	0.11
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG12	4	0.11
(1,1295)	1:75:A:TYR:HA	1:76:A:ILE:HG13	4	0.11
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG2	2	0.11
(1,1244)	1:70:A:LYS:H	1:70:A:LYS:HG3	2	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD11	2	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD12	2	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD13	2	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD11	8	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD12	8	0.11
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD13	8	0.11
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG2	10	0.11
(1,925)	1:57:A:VAL:HG11	1:91:A:GLU:HG3	10	0.11
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG2	10	0.11
(1,925)	1:57:A:VAL:HG12	1:91:A:GLU:HG3	10	0.11
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG2	10	0.11
(1,925)	1:57:A:VAL:HG13	1:91:A:GLU:HG3	10	0.11
(1,791)	1:53:A:VAL:HA	1:74:A:LYS:HA	3	0.11
(1,624)	1:40:A:CYS:HB2	1:41:A:THR:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:40:A:CYS:HB3	1:41:A:THR:H	2	0.11
(1,623)	1:40:A:CYS:HB2	1:41:A:THR:H	2	0.11
(1,623)	1:40:A:CYS:HB3	1:41:A:THR:H	2	0.11
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG21	7	0.11
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG22	7	0.11
(1,533)	1:33:A:GLN:HG2	1:39:A:THR:HG23	7	0.11
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG21	7	0.11
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG22	7	0.11
(1,533)	1:33:A:GLN:HG3	1:39:A:THR:HG23	7	0.11
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG2	8	0.11
(1,459)	1:31:A:GLU:H	1:31:A:GLU:HG3	8	0.11
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD21	6	0.11
(1,423)	1:29:A:ASN:HA	1:29:A:ASN:HD22	6	0.11
(1,290)	1:20:A:ASP:HB2	1:32:A:TRP:HD1	3	0.11
(1,290)	1:20:A:ASP:HB3	1:32:A:TRP:HD1	3	0.11
(1,169)	1:8:A:GLU:H	1:9:A:GLY:H	7	0.11
(1,139)	1:7:A:ASN:HB2	1:45:A:THR:HA	4	0.11
(1,139)	1:7:A:ASN:HB3	1:45:A:THR:HA	4	0.11
(1,138)	1:7:A:ASN:HB2	1:45:A:THR:HA	4	0.11
(1,138)	1:7:A:ASN:HB3	1:45:A:THR:HA	4	0.11
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	2	0.11
(1,51)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	2	0.11
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	2	0.11
(1,51)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	2	0.11
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG12	2	0.11
(1,50)	1:3:A:TYR:HE1	1:5:A:ILE:HG13	2	0.11
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG12	2	0.11
(1,50)	1:3:A:TYR:HE2	1:5:A:ILE:HG13	2	0.11
(1,1444)	1:83:A:PRO:HD2	1:84:A:LYS:H	9	0.1
(1,1444)	1:83:A:PRO:HD3	1:84:A:LYS:H	9	0.1
(1,1443)	1:83:A:PRO:HD2	1:84:A:LYS:H	9	0.1
(1,1443)	1:83:A:PRO:HD3	1:84:A:LYS:H	9	0.1
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG2	1	0.1
(1,1407)	1:80:A:LYS:HA	1:80:A:LYS:HG3	1	0.1
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG2	1	0.1
(1,1406)	1:80:A:LYS:HA	1:80:A:LYS:HG3	1	0.1
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD11	10	0.1
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD12	10	0.1
(1,1134)	1:67:A:ILE:HA	1:67:A:ILE:HD13	10	0.1
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG11	9	0.1
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG12	9	0.1
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG13	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG21	9	0.1
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG22	9	0.1
(1,1121)	1:66:A:ARG:HA	1:77:A:VAL:HG23	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG11	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG12	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG13	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG21	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG22	9	0.1
(1,1120)	1:66:A:ARG:HA	1:77:A:VAL:HG23	9	0.1
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	7	0.1
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	7	0.1
(1,574)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	7	0.1
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	7	0.1
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	7	0.1
(1,574)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	7	0.1
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD11	7	0.1
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD12	7	0.1
(1,573)	1:37:A:CYS:HB2	1:52:A:LEU:HD13	7	0.1
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD11	7	0.1
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD12	7	0.1
(1,573)	1:37:A:CYS:HB3	1:52:A:LEU:HD13	7	0.1
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	7	0.1
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	7	0.1
(1,243)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	7	0.1
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	7	0.1
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	7	0.1
(1,243)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	7	0.1
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD11	7	0.1
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD12	7	0.1
(1,242)	1:18:A:CYS:HB2	1:47:A:ILE:HD13	7	0.1
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD11	7	0.1
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD12	7	0.1
(1,242)	1:18:A:CYS:HB3	1:47:A:ILE:HD13	7	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found