



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:51 AM UTC

PDB ID : 2N8M / pdb_00002n8m
BMRB ID : 25855
Title : Zipcode-binding-protein-1 KH3(DD)KH4 domains in complex with the KH4 RNA target
Authors : Nicastro, G.; Ramos, A.; Candel, A.; Hollingworth, D.
Deposited on : 2015-10-21

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

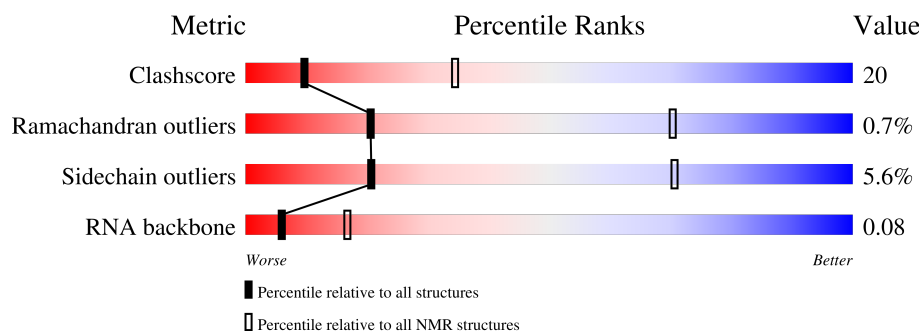
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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
RNA backbone	8273	777

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	191	
2	B	7	

2 Ensemble composition and analysis

This entry contains 12 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:23-A:60, A:67-A:97, A:103-A:142, A:146-A:183 (147)	1.17	2

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 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6
2	9, 10
3	8, 11
Single-model clusters	4; 7; 12

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3150 atoms, of which 1553 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor 2 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			2926	912	1477	261	272	4	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O42254
A	2	ALA	-	expression tag	UNP O42254
A	3	MET	-	expression tag	UNP O42254
A	4	GLY	-	expression tag	UNP O42254
A	14	PHE	TYR	engineered mutation	UNP O42254
A	40	ASP	LYS	engineered mutation	UNP O42254
A	41	ASP	LYS	engineered mutation	UNP O42254

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3').

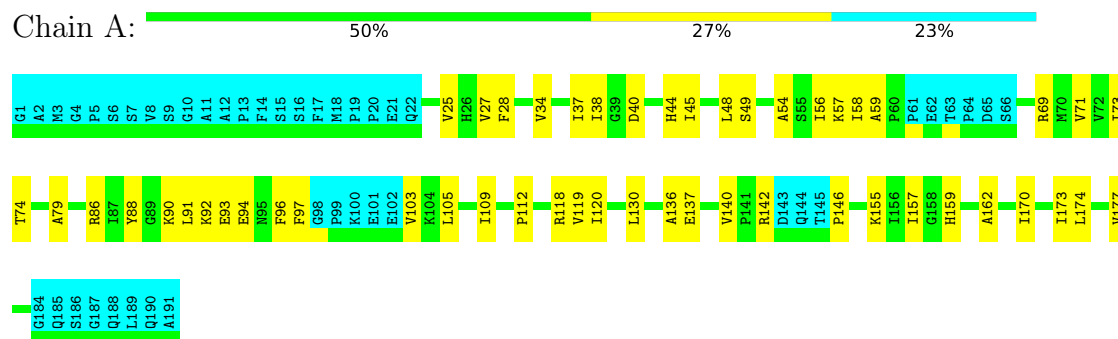
Mol	Chain	Residues	Atoms						Trace
2	B	7	Total	C	H	N	O	P	0
			224	66	76	25	50	7	

4 Residue-property plots [i](#)

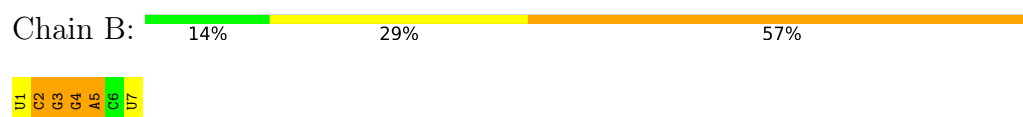
4.1 Average score per residue in the NMR ensemble

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: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

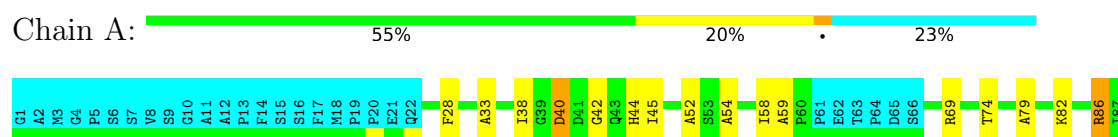


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1





- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

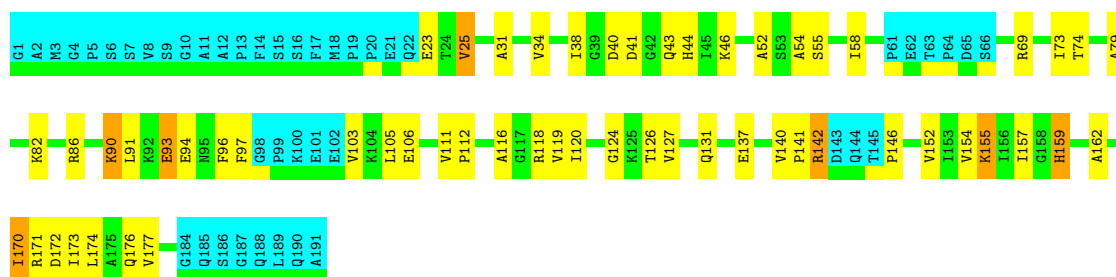
Chain B: 14% 14% 71%



4.2.2 Score per residue for model 2 (medoid)

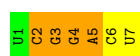
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 47% 26% 23%



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

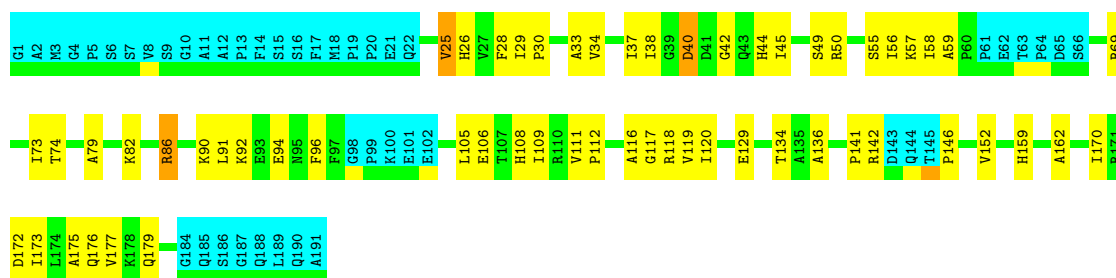
Chain B: 14% 29% 57%



4.2.3 Score per residue for model 3

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 47% 29% 23%

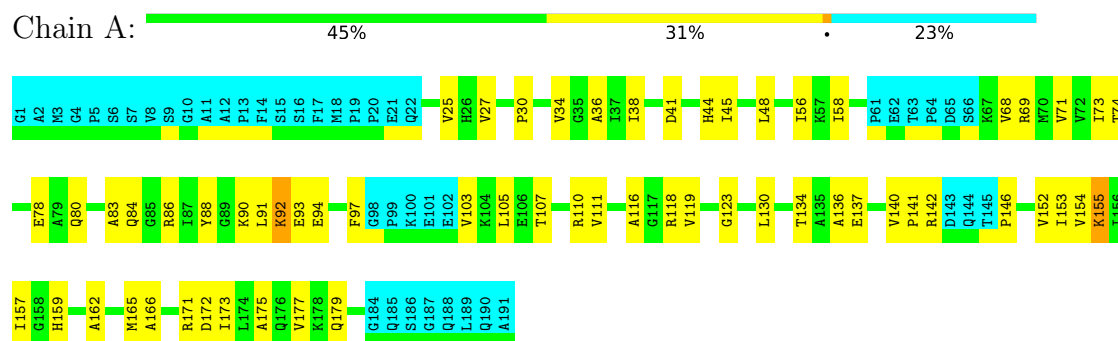


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

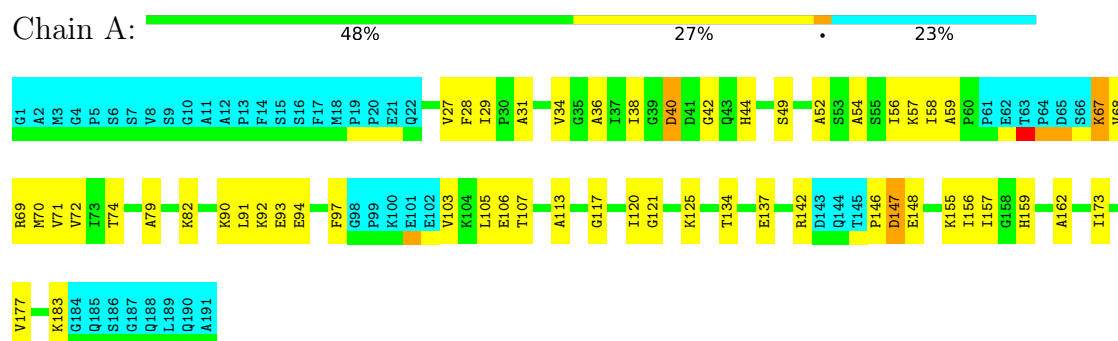


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

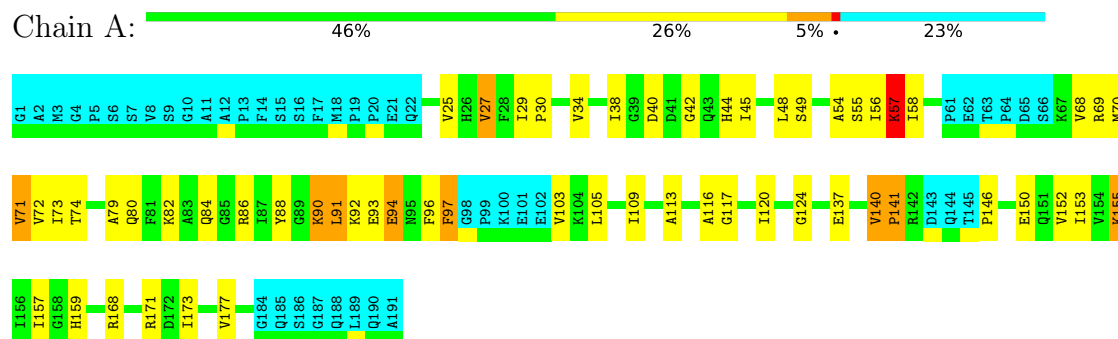


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

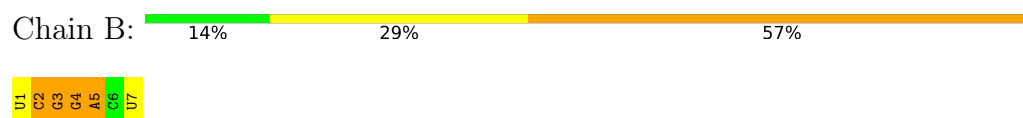


4.2.6 Score per residue for model 6

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

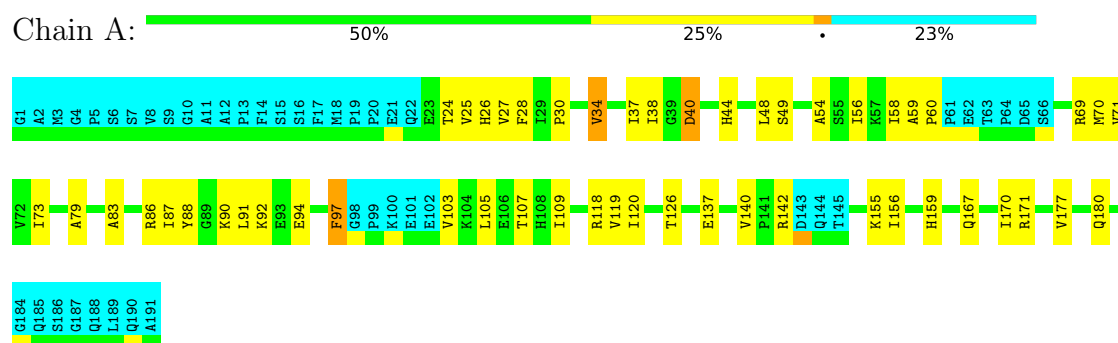


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



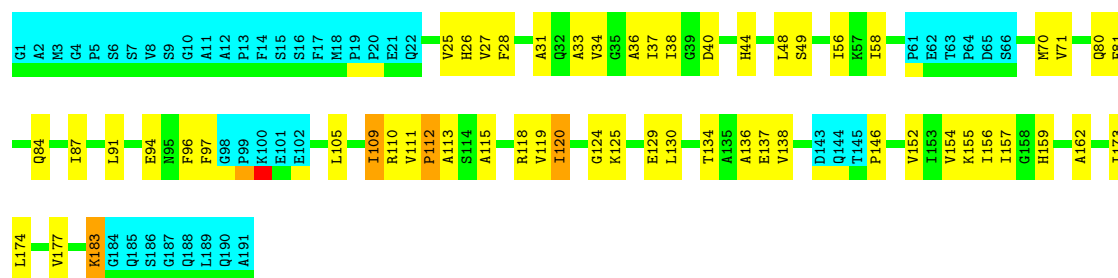
- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.8 Score per residue for model 8

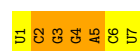
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1





- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

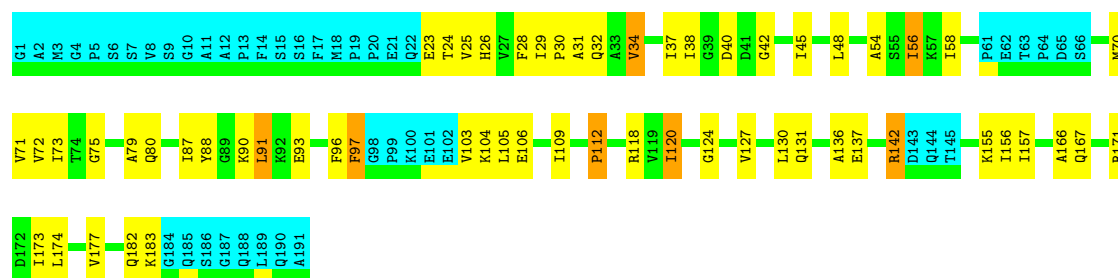
Chain B:



4.2.9 Score per residue for model 9

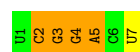
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

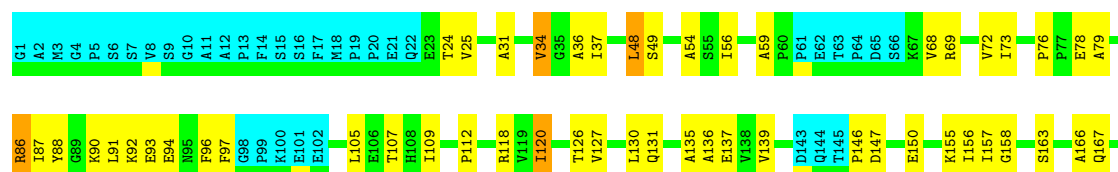
Chain B:

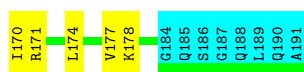


4.2.10 Score per residue for model 10

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:



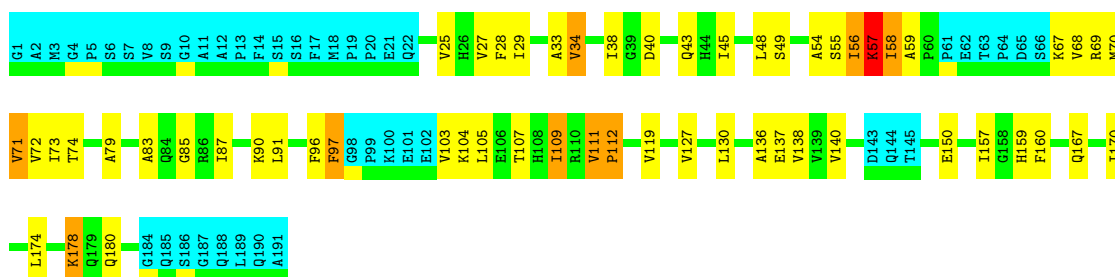


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.11 Score per residue for model 11

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

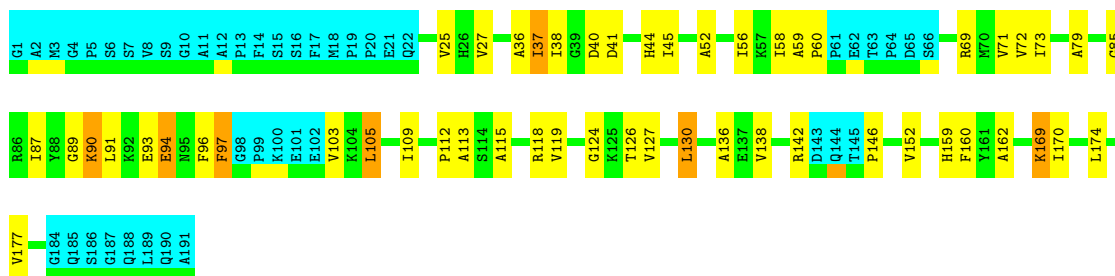


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

Chain B: 29% 14% 57%

U1	C2	G3	G4	A5	C6	U7
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 12 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	refinement	

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	1436
Number of shifts mapped to atoms	1436
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.43±0.02	0±0/1161 (0.0± 0.0%)	0.77±0.03	0±1/1566 (0.0± 0.1%)
2	B	0.25±0.02	0±0/164 (0.0± 0.0%)	0.81±0.04	0±0/253 (0.0± 0.0%)
All	All	0.41	0/15900 (0.0%)	0.77	6/21828 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	3

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	LYS	CA-C-N	5.74	128.33	120.35	6	1
1	A	57	LYS	C-N-CA	5.74	128.33	120.35	6	1
1	A	56	ILE	CA-C-N	5.15	131.11	122.15	11	1
1	A	56	ILE	C-N-CA	5.15	131.11	122.15	11	1
1	A	59	ALA	CA-C-N	5.13	123.35	119.66	3	1
1	A	59	ALA	C-N-CA	5.13	123.35	119.66	3	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	57	LYS	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	67	LYS	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1141	1198	1193	43±10
2	B	148	76	76	9±2
All	All	15468	15288	15228	608

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ALA:HA	1:A:82:LYS:HD2	0.90	1.43	2	2
2:B:4:G:H4'	2:B:5:A:O5'	0.88	1.68	7	12
1:A:130:LEU:HG	1:A:136:ALA:HB3	0.86	1.48	10	3
1:A:56:ILE:HD12	1:A:57:LYS:HG2	0.85	1.46	11	1
1:A:56:ILE:HD12	1:A:57:LYS:HE3	0.81	1.52	6	1
2:B:3:G:H1'	2:B:4:G:N7	0.81	1.91	6	11
1:A:92:LYS:HD2	1:A:97:PHE:HZ	0.80	1.35	10	1
1:A:92:LYS:HD2	1:A:97:PHE:CZ	0.78	2.14	10	2
1:A:40:ASP:HB2	1:A:44:HIS:HB2	0.78	1.52	7	4
1:A:121:GLY:HA3	1:A:125:LYS:HB3	0.76	1.58	5	1
1:A:118:ARG:HG2	1:A:177:VAL:HG22	0.75	1.58	4	3
1:A:58:ILE:HG22	1:A:71:VAL:HA	0.75	1.59	6	1
1:A:48:LEU:HD23	1:A:56:ILE:HD12	0.75	1.58	8	1
1:A:117:GLY:HA3	2:B:4:G:C5	0.75	2.17	3	2
2:B:7:U:O2	2:B:7:U:H2'	0.74	1.83	3	3
1:A:97:PHE:CD1	1:A:103:VAL:HA	0.74	2.17	11	2
1:A:36:ALA:HB1	1:A:94:GLU:HG2	0.74	1.58	5	3
1:A:140:VAL:HG12	1:A:141:PRO:HD2	0.73	1.59	6	1
1:A:34:VAL:HG21	1:A:69:ARG:HD3	0.73	1.59	6	1
1:A:131:GLN:HG3	1:A:137:GLU:HG2	0.73	1.60	1	1
1:A:55:SER:HB2	1:A:74:THR:HB	0.73	1.61	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG12	1:A:109:ILE:HG22	0.73	1.60	11	5
1:A:56:ILE:O	1:A:72:VAL:HB	0.73	1.84	11	2
1:A:134:THR:HG22	1:A:162:ALA:HA	0.72	1.62	4	3
1:A:48:LEU:HD23	1:A:57:LYS:HG3	0.71	1.60	11	1
1:A:159:HIS:H	1:A:162:ALA:HB3	0.71	1.44	4	4
1:A:25:VAL:HG13	1:A:73:ILE:HG23	0.71	1.60	3	1
1:A:91:LEU:HA	1:A:94:GLU:OE2	0.71	1.85	6	1
1:A:49:SER:HB2	1:A:56:ILE:HD13	0.70	1.61	6	1
1:A:48:LEU:HG	1:A:57:LYS:HD2	0.69	1.63	6	1
1:A:34:VAL:HG11	1:A:69:ARG:HD3	0.68	1.63	4	1
1:A:91:LEU:HD11	1:A:105:LEU:HD21	0.68	1.65	2	4
1:A:91:LEU:HD22	1:A:105:LEU:HG	0.68	1.63	12	1
1:A:118:ARG:HD3	1:A:177:VAL:HG22	0.68	1.65	7	1
1:A:120:ILE:HG12	1:A:124:GLY:HA2	0.67	1.66	6	1
1:A:57:LYS:HA	1:A:72:VAL:H	0.67	1.49	11	2
1:A:118:ARG:HG2	1:A:177:VAL:CG2	0.67	2.19	10	5
1:A:141:PRO:HD3	1:A:153:ILE:O	0.67	1.89	6	1
1:A:118:ARG:HG2	1:A:177:VAL:HG21	0.66	1.66	10	3
1:A:56:ILE:HG12	1:A:73:ILE:HD13	0.66	1.63	3	1
1:A:107:THR:HG21	1:A:167:GLN:HE21	0.66	1.48	11	1
1:A:141:PRO:HG3	1:A:152:VAL:HB	0.65	1.66	3	1
1:A:34:VAL:HG21	1:A:69:ARG:HB3	0.65	1.69	4	1
1:A:104:LYS:HD2	1:A:157:ILE:HG22	0.65	1.69	9	1
1:A:90:LYS:O	1:A:94:GLU:HG3	0.65	1.91	6	1
1:A:40:ASP:HB3	1:A:44:HIS:HB2	0.64	1.69	1	2
1:A:112:PRO:HG2	1:A:174:LEU:HD22	0.64	1.67	9	2
1:A:91:LEU:CD2	1:A:105:LEU:HG	0.64	2.23	12	1
1:A:91:LEU:HA	1:A:96:PHE:CD1	0.63	2.27	12	1
1:A:56:ILE:CD1	1:A:57:LYS:HG2	0.63	2.23	11	1
1:A:130:LEU:HB3	1:A:136:ALA:HB3	0.63	1.69	11	2
1:A:169:LYS:HE3	1:A:169:LYS:HA	0.63	1.70	12	1
1:A:91:LEU:HD22	1:A:96:PHE:CE2	0.62	2.29	11	3
2:B:1:U:H3'	2:B:1:U:O2	0.62	1.94	6	1
1:A:88:TYR:CE1	1:A:105:LEU:HG	0.62	2.30	1	4
1:A:48:LEU:CG	1:A:57:LYS:HD2	0.62	2.24	6	1
1:A:27:VAL:HG12	1:A:71:VAL:HG22	0.62	1.72	7	3
1:A:25:VAL:HG13	1:A:73:ILE:HB	0.61	1.72	2	1
1:A:49:SER:N	1:A:56:ILE:HD13	0.61	2.10	11	1
1:A:120:ILE:HD13	1:A:127:VAL:HG23	0.61	1.73	2	1
2:B:7:U:O2	2:B:7:U:C2'	0.61	2.48	10	3
1:A:57:LYS:HE2	1:A:72:VAL:O	0.61	1.96	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:VAL:HG13	1:A:159:HIS:HD2	0.61	1.56	12	1
1:A:103:VAL:HG13	1:A:159:HIS:CD2	0.61	2.31	12	1
2:B:1:U:O2	2:B:1:U:H2'	0.60	1.95	8	2
1:A:91:LEU:HD22	1:A:105:LEU:CG	0.60	2.26	12	1
1:A:38:ILE:HD11	1:A:69:ARG:HH11	0.60	1.56	7	1
1:A:91:LEU:HB3	1:A:97:PHE:CE2	0.60	2.31	7	1
1:A:38:ILE:O	1:A:42:GLY:HA2	0.60	1.96	5	5
1:A:97:PHE:CD2	1:A:103:VAL:HG12	0.60	2.31	2	3
1:A:136:ALA:HA	1:A:157:ILE:O	0.60	1.97	8	2
1:A:54:ALA:HB2	1:A:79:ALA:HB1	0.60	1.71	7	6
1:A:27:VAL:O	1:A:70:MET:HA	0.60	1.96	5	1
1:A:97:PHE:CD2	1:A:103:VAL:HA	0.60	2.30	9	1
1:A:106:GLU:HG3	1:A:157:ILE:HD11	0.59	1.72	2	1
1:A:91:LEU:CD1	1:A:105:LEU:HD11	0.59	2.27	11	3
1:A:116:ALA:HB2	1:A:152:VAL:HG21	0.59	1.74	4	3
1:A:45:ILE:HG12	1:A:58:ILE:HG21	0.59	1.73	3	2
1:A:136:ALA:HB1	1:A:166:ALA:HB2	0.59	1.75	9	2
1:A:91:LEU:HA	1:A:94:GLU:CD	0.59	2.21	6	1
2:B:1:U:C2'	2:B:1:U:O2	0.59	2.50	7	1
1:A:173:ILE:O	1:A:177:VAL:HG23	0.59	1.98	4	6
1:A:134:THR:HG21	1:A:165:MET:HB3	0.59	1.75	4	1
1:A:105:LEU:O	1:A:157:ILE:HA	0.58	1.98	5	3
1:A:28:PHE:HB2	1:A:106:GLU:HG3	0.58	1.73	5	3
1:A:34:VAL:HG13	1:A:69:ARG:HE	0.58	1.56	2	1
1:A:167:GLN:O	1:A:171:ARG:HG2	0.58	1.98	9	2
1:A:34:VAL:HG21	1:A:69:ARG:HB2	0.58	1.75	3	2
1:A:73:ILE:HG21	1:A:80:GLN:HG2	0.58	1.74	4	1
1:A:48:LEU:HB3	1:A:56:ILE:HG21	0.58	1.76	10	1
1:A:56:ILE:HA	1:A:72:VAL:O	0.57	1.99	5	4
1:A:136:ALA:HB2	1:A:162:ALA:HB1	0.57	1.76	12	3
1:A:123:GLY:HA3	2:B:4:G:OP1	0.57	1.98	4	1
1:A:91:LEU:HD11	1:A:105:LEU:HD11	0.57	1.75	10	2
1:A:127:VAL:O	1:A:131:GLN:HB3	0.57	2.00	10	1
1:A:103:VAL:O	1:A:159:HIS:HA	0.57	1.99	11	1
1:A:29:ILE:HG13	1:A:34:VAL:HG22	0.57	1.77	6	2
1:A:52:ALA:HA	1:A:82:LYS:HD3	0.57	1.77	5	1
1:A:45:ILE:HD11	1:A:57:LYS:HB2	0.57	1.76	11	1
1:A:45:ILE:HG12	1:A:58:ILE:CG2	0.57	2.30	4	3
1:A:34:VAL:O	1:A:38:ILE:HG12	0.57	1.99	5	5
1:A:137:GLU:O	1:A:156:ILE:HA	0.57	2.00	7	5
1:A:25:VAL:HG13	1:A:73:ILE:CG2	0.56	2.30	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:GLY:HA3	2:B:4:G:N7	0.56	2.14	5	1
1:A:56:ILE:HA	1:A:57:LYS:HE3	0.56	1.76	6	1
1:A:58:ILE:HG13	1:A:69:ARG:HD3	0.56	1.76	11	1
1:A:113:ALA:CB	1:A:146:PRO:HB3	0.55	2.31	5	3
1:A:87:ILE:O	1:A:91:LEU:HG	0.55	2.00	8	4
1:A:167:GLN:O	1:A:171:ARG:HG3	0.55	2.02	7	1
1:A:80:GLN:O	1:A:84:GLN:HB2	0.55	2.00	4	1
1:A:97:PHE:HB2	1:A:103:VAL:HG12	0.55	1.78	6	1
1:A:56:ILE:HA	1:A:57:LYS:CE	0.55	2.32	6	2
1:A:91:LEU:HB3	1:A:96:PHE:HB2	0.55	1.77	9	1
1:A:73:ILE:HD12	1:A:83:ALA:HB1	0.55	1.79	11	1
2:B:2:C:C5'	2:B:3:G:OP1	0.55	2.55	9	12
2:B:2:C:H5''	2:B:3:G:OP1	0.55	2.01	6	7
1:A:94:GLU:OE2	1:A:96:PHE:HD2	0.55	1.84	6	1
1:A:113:ALA:HB1	1:A:146:PRO:HB3	0.54	1.78	5	1
1:A:81:PHE:HA	1:A:84:GLN:HE21	0.54	1.62	8	1
1:A:171:ARG:HG3	1:A:172:ASP:N	0.54	2.17	4	2
1:A:57:LYS:HD3	1:A:73:ILE:CD1	0.54	2.32	6	1
1:A:80:GLN:O	1:A:84:GLN:HB3	0.54	2.03	6	1
1:A:171:ARG:HD3	1:A:174:LEU:HD12	0.54	1.80	10	1
1:A:139:VAL:HB	1:A:155:LYS:CG	0.54	2.32	10	1
1:A:90:LYS:HA	1:A:93:GLU:HG2	0.54	1.79	1	6
1:A:26:HIS:HA	1:A:71:VAL:O	0.54	2.03	9	3
1:A:90:LYS:N	1:A:90:LYS:HD2	0.53	2.18	12	1
1:A:58:ILE:HG13	1:A:58:ILE:O	0.53	2.02	4	2
2:B:4:G:H4'	2:B:5:A:O4'	0.53	2.03	10	3
1:A:45:ILE:O	1:A:56:ILE:HD11	0.53	2.04	6	2
1:A:23:GLU:HG3	1:A:80:GLN:NE2	0.53	2.18	9	1
1:A:90:LYS:O	1:A:94:GLU:HB2	0.53	2.04	12	1
1:A:34:VAL:HG11	1:A:69:ARG:HD2	0.53	1.79	3	1
1:A:146:PRO:HB2	1:A:150:GLU:HA	0.53	1.79	6	1
1:A:58:ILE:HB	1:A:70:MET:O	0.53	2.03	11	1
2:B:1:U:O2	2:B:1:U:C3'	0.53	2.56	6	1
2:B:4:G:H4'	2:B:5:A:C5'	0.53	2.34	1	9
1:A:107:THR:O	1:A:155:LYS:HA	0.53	2.04	10	4
1:A:57:LYS:HD3	1:A:73:ILE:HD13	0.52	1.81	11	2
1:A:117:GLY:HA3	2:B:4:G:C6	0.52	2.39	3	1
1:A:91:LEU:HD12	1:A:103:VAL:HB	0.52	1.81	5	1
1:A:28:PHE:HB3	1:A:68:VAL:HB	0.52	1.80	11	1
1:A:120:ILE:HD13	1:A:140:VAL:HG23	0.52	1.81	7	1
1:A:118:ARG:HG3	1:A:173:ILE:CG2	0.52	2.35	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ALA:HB1	1:A:79:ALA:HA	0.52	1.81	12	1
1:A:36:ALA:CB	1:A:94:GLU:HG2	0.52	2.34	5	2
1:A:28:PHE:HA	1:A:69:ARG:O	0.52	2.04	11	1
1:A:27:VAL:HG12	1:A:71:VAL:CG2	0.52	2.34	7	2
1:A:29:ILE:HG12	1:A:69:ARG:NE	0.51	2.20	11	1
1:A:172:ASP:O	1:A:176:GLN:HG2	0.51	2.04	3	1
1:A:41:ASP:HB3	1:A:44:HIS:HB2	0.51	1.80	2	3
1:A:91:LEU:HD21	1:A:105:LEU:HD11	0.51	1.81	9	2
1:A:94:GLU:CD	1:A:96:PHE:CD2	0.51	2.87	6	1
1:A:146:PRO:HB3	1:A:150:GLU:HA	0.51	1.82	10	1
1:A:82:LYS:O	1:A:86:ARG:HB2	0.51	2.05	6	2
1:A:94:GLU:HG2	1:A:96:PHE:CE2	0.51	2.40	3	2
1:A:178:LYS:HA	1:A:178:LYS:HE2	0.51	1.82	11	1
1:A:59:ALA:HB1	1:A:69:ARG:HD2	0.51	1.83	5	1
1:A:27:VAL:HG13	1:A:71:VAL:CG2	0.51	2.36	6	1
1:A:31:ALA:O	1:A:34:VAL:HG22	0.51	2.06	9	3
1:A:27:VAL:HG13	1:A:71:VAL:HG22	0.51	1.81	6	2
1:A:91:LEU:HD22	1:A:96:PHE:CD2	0.51	2.41	10	3
1:A:110:ARG:HH11	1:A:110:ARG:HG3	0.51	1.64	8	1
1:A:172:ASP:O	1:A:176:GLN:HG3	0.51	2.06	2	1
1:A:56:ILE:HA	1:A:57:LYS:HE2	0.51	1.81	11	1
1:A:90:LYS:O	1:A:93:GLU:HG2	0.51	2.06	4	2
1:A:119:VAL:HG11	1:A:154:VAL:HG11	0.51	1.83	4	1
2:B:1:U:O2	2:B:1:U:C2'	0.50	2.58	8	2
1:A:116:ALA:O	1:A:119:VAL:HG12	0.50	2.06	4	3
2:B:4:G:N3	2:B:4:G:H2'	0.50	2.21	4	5
1:A:58:ILE:HG12	1:A:59:ALA:N	0.50	2.21	11	1
1:A:91:LEU:HB2	1:A:103:VAL:HG11	0.50	1.83	1	1
1:A:170:ILE:O	1:A:174:LEU:HG	0.50	2.06	11	2
1:A:182:GLN:HG3	1:A:183:LYS:HG3	0.50	1.84	9	1
1:A:178:LYS:HA	1:A:178:LYS:CE	0.50	2.36	11	1
2:B:1:U:O5'	2:B:2:C:H3'	0.50	2.07	6	1
1:A:28:PHE:CE2	1:A:70:MET:HB3	0.50	2.42	7	3
1:A:137:GLU:HB3	1:A:157:ILE:HB	0.49	1.83	4	3
1:A:112:PRO:HD2	1:A:174:LEU:HD13	0.49	1.84	8	1
1:A:33:ALA:HB1	1:A:96:PHE:CE2	0.49	2.41	11	1
1:A:91:LEU:HD12	1:A:96:PHE:CD2	0.49	2.42	9	1
1:A:58:ILE:HG22	1:A:71:VAL:HG12	0.49	1.83	12	1
1:A:127:VAL:HG22	1:A:138:VAL:HB	0.49	1.83	12	1
1:A:150:GLU:O	1:A:150:GLU:HG3	0.49	2.05	11	1
1:A:124:GLY:HA3	2:B:5:A:O2'	0.49	2.06	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LYS:HB3	1:A:157:ILE:HD11	0.49	1.84	9	1
1:A:118:ARG:CG	1:A:177:VAL:HG21	0.49	2.37	3	1
1:A:27:VAL:HB	1:A:71:VAL:CG2	0.49	2.37	12	1
1:A:118:ARG:HG3	1:A:173:ILE:HG22	0.49	1.83	8	1
1:A:104:LYS:HD3	1:A:157:ILE:CG2	0.49	2.38	11	1
1:A:134:THR:CG2	1:A:162:ALA:HA	0.49	2.37	3	2
1:A:24:THR:HA	1:A:73:ILE:O	0.49	2.08	10	3
2:B:6:C:C4	2:B:7:U:C5	0.48	3.01	1	1
1:A:33:ALA:HB1	1:A:96:PHE:CZ	0.48	2.43	11	2
1:A:146:PRO:HB3	1:A:152:VAL:HG13	0.48	1.85	8	1
1:A:59:ALA:O	1:A:69:ARG:HD2	0.48	2.07	10	3
1:A:142:ARG:HB2	2:B:5:A:H62	0.48	1.68	4	2
1:A:94:GLU:CD	1:A:96:PHE:HD2	0.48	2.16	6	1
1:A:87:ILE:O	1:A:91:LEU:HD22	0.48	2.08	9	1
1:A:142:ARG:HG3	2:B:4:G:H21	0.48	1.67	5	1
1:A:112:PRO:CD	1:A:174:LEU:HD21	0.48	2.39	1	1
1:A:25:VAL:CG2	1:A:73:ILE:HB	0.48	2.39	11	2
1:A:25:VAL:HB	1:A:73:ILE:HB	0.48	1.86	12	1
1:A:91:LEU:HB3	1:A:97:PHE:CE1	0.48	2.43	5	1
1:A:36:ALA:O	1:A:40:ASP:HB2	0.48	2.08	12	1
1:A:111:VAL:HG11	1:A:170:ILE:HD11	0.47	1.83	2	1
1:A:58:ILE:HG22	1:A:71:VAL:CA	0.47	2.34	6	1
1:A:146:PRO:CB	1:A:150:GLU:HA	0.47	2.38	6	2
2:B:3:G:N3	2:B:4:G:C6	0.47	2.81	8	2
1:A:120:ILE:HD13	1:A:124:GLY:HA2	0.47	1.85	8	2
1:A:37:ILE:HD11	1:A:87:ILE:HA	0.47	1.85	12	1
1:A:126:THR:O	1:A:130:LEU:HB2	0.47	2.08	12	1
1:A:112:PRO:HD2	1:A:174:LEU:HD11	0.47	1.84	1	3
1:A:30:PRO:O	1:A:34:VAL:HG23	0.47	2.10	6	2
1:A:27:VAL:O	1:A:71:VAL:HG13	0.47	2.10	11	1
1:A:85:GLY:HA2	1:A:160:PHE:CE1	0.47	2.44	11	2
1:A:90:LYS:O	1:A:93:GLU:HG3	0.47	2.09	2	1
2:B:5:A:H2'	2:B:6:C:O4'	0.47	2.10	7	3
1:A:40:ASP:HB2	1:A:44:HIS:CB	0.47	2.39	5	2
1:A:28:PHE:CE2	1:A:106:GLU:HB3	0.47	2.45	1	1
1:A:38:ILE:HD11	1:A:58:ILE:HD13	0.47	1.86	6	1
1:A:58:ILE:HB	1:A:69:ARG:HD2	0.47	1.86	7	1
1:A:86:ARG:NE	1:A:86:ARG:HA	0.47	2.25	7	1
1:A:38:ILE:HD12	1:A:45:ILE:HG21	0.47	1.87	3	1
2:B:6:C:O2'	2:B:7:U:H5'	0.47	2.10	4	1
1:A:131:GLN:HG2	1:A:137:GLU:HG3	0.47	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD21	1:A:166:ALA:HA	0.46	1.86	4	1
1:A:120:ILE:HD11	1:A:124:GLY:HA2	0.46	1.86	2	1
1:A:140:VAL:HB	1:A:141:PRO:HD2	0.46	1.86	2	2
1:A:127:VAL:O	1:A:131:GLN:HB2	0.46	2.09	9	1
1:A:142:ARG:HB2	2:B:5:A:N6	0.46	2.25	4	1
1:A:155:LYS:N	1:A:155:LYS:HD2	0.46	2.26	6	1
1:A:73:ILE:HD12	1:A:83:ALA:CB	0.46	2.39	11	1
1:A:88:TYR:O	1:A:92:LYS:HG2	0.46	2.10	10	1
1:A:85:GLY:HA2	1:A:160:PHE:HE1	0.46	1.70	11	1
1:A:58:ILE:HB	1:A:70:MET:C	0.46	2.35	11	1
1:A:119:VAL:CG2	1:A:170:ILE:HB	0.46	2.41	3	1
1:A:120:ILE:HD13	1:A:120:ILE:O	0.46	2.10	8	2
2:B:6:C:H2'	2:B:7:U:O4'	0.46	2.10	1	1
1:A:45:ILE:HG12	1:A:58:ILE:HD13	0.46	1.88	12	1
1:A:54:ALA:HB2	1:A:79:ALA:CB	0.46	2.41	1	2
2:B:5:A:O5'	2:B:5:A:H8	0.46	1.94	7	1
1:A:111:VAL:HG23	1:A:174:LEU:HD22	0.46	1.87	11	1
1:A:49:SER:HB2	1:A:56:ILE:HB	0.45	1.88	11	2
1:A:141:PRO:CG	1:A:152:VAL:HB	0.45	2.40	3	1
1:A:156:ILE:HD11	1:A:170:ILE:HD13	0.45	1.87	10	1
1:A:111:VAL:HG12	1:A:174:LEU:HD11	0.45	1.86	8	1
1:A:49:SER:HB2	1:A:56:ILE:HG22	0.45	1.89	10	1
1:A:96:PHE:HB3	1:A:97:PHE:CD2	0.45	2.47	1	1
1:A:135:ALA:O	1:A:158:GLY:HA3	0.45	2.10	10	1
2:B:5:A:C6	2:B:6:C:N3	0.45	2.85	1	1
1:A:112:PRO:HA	1:A:150:GLU:O	0.45	2.11	11	1
1:A:86:ARG:C	1:A:86:ARG:HD3	0.45	2.37	10	3
1:A:41:ASP:CB	1:A:44:HIS:HB2	0.45	2.42	2	1
1:A:120:ILE:HA	1:A:126:THR:OG1	0.45	2.11	2	1
1:A:109:ILE:HG12	1:A:154:VAL:HG23	0.45	1.87	8	1
1:A:140:VAL:HG12	1:A:154:VAL:HG12	0.45	1.88	4	1
1:A:37:ILE:O	1:A:44:HIS:HB3	0.45	2.11	12	2
1:A:57:LYS:CD	1:A:73:ILE:HD13	0.45	2.42	11	1
2:B:3:G:H1'	2:B:4:G:C5	0.45	2.47	6	3
1:A:56:ILE:CD1	1:A:57:LYS:H	0.45	2.25	11	1
1:A:56:ILE:CG1	1:A:57:LYS:H	0.45	2.24	11	1
1:A:58:ILE:O	1:A:60:PRO:HD3	0.45	2.12	12	1
1:A:26:HIS:O	1:A:108:HIS:HB2	0.44	2.12	3	1
1:A:112:PRO:CG	1:A:174:LEU:HD22	0.44	2.41	9	1
1:A:31:ALA:HA	1:A:34:VAL:HG23	0.44	1.88	2	2
1:A:120:ILE:HD13	1:A:127:VAL:CG2	0.44	2.42	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LYS:O	1:A:90:LYS:HD3	0.44	2.12	1	5
1:A:111:VAL:HB	1:A:112:PRO:HD2	0.44	1.88	3	1
1:A:125:LYS:O	1:A:129:GLU:HG3	0.44	2.13	8	1
2:B:4:G:O2'	2:B:5:A:C8	0.44	2.67	11	1
1:A:40:ASP:HB3	1:A:44:HIS:HB3	0.44	1.90	2	1
1:A:142:ARG:HG3	2:B:5:A:H62	0.44	1.73	9	1
1:A:120:ILE:O	1:A:126:THR:HB	0.44	2.12	10	1
1:A:117:GLY:O	1:A:120:ILE:HG22	0.44	2.13	6	2
1:A:30:PRO:HA	1:A:68:VAL:HG12	0.44	1.89	4	1
1:A:33:ALA:HB1	1:A:91:LEU:HD22	0.44	1.90	1	1
1:A:79:ALA:HA	1:A:82:LYS:HG2	0.44	1.87	3	1
1:A:56:ILE:HD12	1:A:57:LYS:H	0.44	1.72	11	1
1:A:142:ARG:HG2	2:B:5:A:H62	0.44	1.72	2	1
1:A:50:ARG:N	1:A:50:ARG:HD2	0.44	2.27	3	1
1:A:86:ARG:O	1:A:86:ARG:HD3	0.44	2.13	3	1
1:A:119:VAL:HG12	1:A:138:VAL:HG11	0.44	1.87	8	2
1:A:140:VAL:CG1	1:A:141:PRO:HD2	0.44	2.38	6	1
1:A:91:LEU:CD1	1:A:105:LEU:HD21	0.43	2.43	1	1
2:B:1:U:O2	2:B:1:U:O4'	0.43	2.36	5	1
1:A:68:VAL:C	1:A:69:ARG:HD2	0.43	2.38	6	1
1:A:127:VAL:HG13	1:A:137:GLU:HA	0.43	1.88	11	1
1:A:175:ALA:O	1:A:179:GLN:HG3	0.43	2.13	3	2
1:A:112:PRO:HG3	1:A:178:LYS:HD3	0.43	1.88	10	1
1:A:30:PRO:HG2	1:A:97:PHE:CZ	0.43	2.48	7	1
1:A:49:SER:HB3	1:A:56:ILE:CG2	0.43	2.44	7	1
1:A:29:ILE:O	1:A:68:VAL:HB	0.43	2.12	5	1
1:A:90:LYS:HA	1:A:93:GLU:CG	0.43	2.43	5	1
1:A:67:LYS:HB3	1:A:67:LYS:NZ	0.43	2.28	11	1
1:A:73:ILE:CG2	1:A:80:GLN:HG2	0.43	2.43	4	1
1:A:34:VAL:CG1	1:A:69:ARG:HD3	0.43	2.43	7	1
1:A:28:PHE:HB2	1:A:106:GLU:CG	0.43	2.43	3	1
1:A:49:SER:HB3	1:A:56:ILE:HG22	0.43	1.88	7	2
1:A:56:ILE:O	1:A:72:VAL:CB	0.43	2.63	11	1
1:A:157:ILE:HD12	1:A:157:ILE:N	0.43	2.29	2	1
1:A:33:ALA:HA	1:A:96:PHE:CE2	0.43	2.49	3	1
1:A:38:ILE:HD11	1:A:58:ILE:CD1	0.43	2.43	6	1
1:A:120:ILE:HG12	2:B:5:A:C2	0.43	2.48	7	1
1:A:23:GLU:HB3	1:A:75:GLY:O	0.43	2.13	9	1
1:A:86:ARG:HD3	1:A:86:ARG:O	0.43	2.13	1	1
1:A:120:ILE:HD13	1:A:140:VAL:HG13	0.43	1.91	1	1
1:A:29:ILE:HG22	1:A:105:LEU:HD13	0.43	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LYS:N	1:A:155:LYS:HD3	0.43	2.28	4	1
1:A:168:ARG:O	1:A:171:ARG:HG2	0.43	2.14	6	1
1:A:38:ILE:HD11	1:A:69:ARG:NH1	0.43	2.27	7	1
1:A:80:GLN:O	1:A:84:GLN:HG2	0.43	2.14	8	1
1:A:48:LEU:HD23	1:A:56:ILE:CD1	0.43	2.43	9	1
1:A:119:VAL:HG13	1:A:170:ILE:HG12	0.43	1.90	7	1
1:A:37:ILE:HD13	1:A:90:LYS:HG3	0.43	1.90	3	1
1:A:56:ILE:C	1:A:72:VAL:HB	0.43	2.39	11	1
2:B:5:A:C5	2:B:6:C:C4	0.42	3.07	1	1
1:A:34:VAL:HG13	1:A:69:ARG:HG2	0.42	1.90	11	1
1:A:140:VAL:HG22	2:B:5:A:C2	0.42	2.48	11	1
1:A:87:ILE:HG22	1:A:105:LEU:HD11	0.42	1.90	12	1
1:A:58:ILE:HA	1:A:70:MET:O	0.42	2.14	6	2
2:B:1:U:O2	2:B:1:U:H5''	0.42	2.14	8	1
1:A:31:ALA:HB2	1:A:68:VAL:C	0.42	2.40	10	1
1:A:147:ASP:OD1	1:A:148:GLU:HG2	0.42	2.14	5	1
1:A:112:PRO:HG2	1:A:115:ALA:HB3	0.42	1.91	1	2
1:A:91:LEU:HD22	1:A:105:LEU:CD1	0.42	2.44	12	1
2:B:4:G:C4'	2:B:5:A:O5'	0.42	2.60	5	3
1:A:45:ILE:HD11	1:A:56:ILE:HG21	0.42	1.91	4	1
1:A:140:VAL:HG12	1:A:154:VAL:HG22	0.42	1.91	2	1
1:A:37:ILE:HG22	1:A:38:ILE:HD13	0.42	1.91	8	1
1:A:160:PHE:O	1:A:164:GLN:HG2	0.42	2.15	1	1
1:A:118:ARG:HG3	1:A:177:VAL:HG21	0.42	1.90	3	1
1:A:59:ALA:CB	1:A:70:MET:HG2	0.42	2.45	7	1
1:A:37:ILE:HD13	1:A:90:LYS:HD2	0.42	1.90	9	2
1:A:38:ILE:HG23	1:A:45:ILE:HG21	0.42	1.91	9	1
1:A:38:ILE:HD11	1:A:58:ILE:HD12	0.42	1.92	11	1
1:A:57:LYS:HA	1:A:72:VAL:N	0.41	2.24	11	1
1:A:38:ILE:HD13	1:A:45:ILE:HB	0.41	1.92	12	1
1:A:113:ALA:HB2	1:A:146:PRO:HB3	0.41	1.91	12	1
1:A:97:PHE:CD1	1:A:103:VAL:HG12	0.41	2.49	1	1
1:A:43:GLN:HG2	1:A:46:LYS:HB2	0.41	1.91	2	1
1:A:120:ILE:HA	1:A:126:THR:HG1	0.41	1.74	2	1
1:A:111:VAL:HG23	1:A:152:VAL:HG23	0.41	1.91	4	1
2:B:4:G:O2'	2:B:5:A:P	0.41	2.78	4	1
1:A:25:VAL:HG22	1:A:73:ILE:HB	0.41	1.91	10	1
1:A:25:VAL:HG12	1:A:109:ILE:CG2	0.41	2.45	6	2
1:A:119:VAL:HG13	1:A:170:ILE:HB	0.41	1.91	12	1
2:B:4:G:HO2'	2:B:5:A:P	0.41	2.38	12	1
1:A:113:ALA:CB	1:A:152:VAL:HG13	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLY:O	1:A:93:GLU:HG2	0.41	2.16	12	1
1:A:91:LEU:HB3	1:A:103:VAL:CG1	0.41	2.46	6	1
1:A:163:SER:O	1:A:167:GLN:HG3	0.41	2.15	10	1
1:A:37:ILE:HD13	1:A:37:ILE:HA	0.41	1.76	12	1
1:A:105:LEU:HD23	1:A:105:LEU:HA	0.41	1.74	12	1
1:A:57:LYS:HA	1:A:72:VAL:HB	0.41	1.92	6	1
1:A:138:VAL:HA	1:A:155:LYS:O	0.41	2.15	8	1
1:A:92:LYS:NZ	1:A:92:LYS:HB3	0.41	2.30	4	1
1:A:83:ALA:O	1:A:87:ILE:HG13	0.41	2.16	7	1
1:A:97:PHE:HD2	1:A:103:VAL:HG12	0.41	1.73	7	1
1:A:120:ILE:CD1	1:A:124:GLY:HA2	0.41	2.44	8	1
1:A:29:ILE:HB	1:A:30:PRO:CD	0.41	2.46	9	1
1:A:58:ILE:HG13	1:A:69:ARG:CD	0.41	2.44	11	1
1:A:155:LYS:HD2	1:A:155:LYS:N	0.40	2.30	2	1
1:A:110:ARG:HH11	1:A:153:ILE:HD11	0.40	1.76	4	1
1:A:88:TYR:HA	1:A:91:LEU:CD2	0.40	2.46	9	1
1:A:97:PHE:CZ	1:A:103:VAL:CG1	0.40	3.04	4	1
1:A:76:PRO:HD2	1:A:79:ALA:HB3	0.40	1.93	10	1
1:A:56:ILE:CA	1:A:57:LYS:HE2	0.40	2.47	11	1
1:A:169:LYS:HE3	1:A:169:LYS:CA	0.40	2.44	12	1
1:A:23:GLU:O	1:A:74:THR:HA	0.40	2.17	2	1
1:A:83:ALA:O	1:A:86:ARG:HB3	0.40	2.17	4	1
1:A:29:ILE:HB	1:A:30:PRO:HD2	0.40	1.91	9	1
1:A:130:LEU:HD21	1:A:166:ALA:CB	0.40	2.46	4	1
1:A:90:LYS:O	1:A:94:GLU:HG2	0.40	2.16	7	1
1:A:115:ALA:HB1	1:A:177:VAL:HG11	0.40	1.92	8	1
1:A:34:VAL:HG21	1:A:69:ARG:CB	0.40	2.45	4	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	147/191 (77%)	140±2 (95±1%)	6±2 (4±1%)	1±1 (1±1%)	20	70
All	All	1764/2292 (77%)	1680 (95%)	71 (4%)	13 (1%)	20	70

All 5 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	40	ASP	6
1	A	112	PRO	3
1	A	183	LYS	2
1	A	147	ASP	1
1	A	141	PRO	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	120/154 (78%)	113±2 (94±2%)	7±2 (6±2%)	21	70
All	All	1440/1848 (78%)	1360 (94%)	80 (6%)	21	70

All 39 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	97	PHE	5
1	A	159	HIS	4
1	A	109	ILE	4
1	A	58	ILE	4
1	A	120	ILE	4
1	A	34	VAL	4
1	A	86	ARG	3
1	A	25	VAL	3
1	A	90	LYS	3
1	A	142	ARG	3
1	A	155	LYS	3
1	A	57	LYS	3
1	A	91	LEU	3
1	A	92	LYS	3
1	A	48	LEU	3
1	A	71	VAL	3
1	A	78	GLU	2
1	A	94	GLU	2
1	A	88	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	GLU	1
1	A	170	ILE	1
1	A	129	GLU	1
1	A	49	SER	1
1	A	27	VAL	1
1	A	140	VAL	1
1	A	126	THR	1
1	A	134	THR	1
1	A	183	LYS	1
1	A	32	GLN	1
1	A	56	ILE	1
1	A	147	ASP	1
1	A	43	GLN	1
1	A	111	VAL	1
1	A	178	LYS	1
1	A	37	ILE	1
1	A	105	LEU	1
1	A	130	LEU	1
1	A	152	VAL	1
1	A	169	LYS	1

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	6/7 (86%)	5±0 (83±0%)	2±1 (38±12%)	0.27±0.00
All	All	74/84 (88%)	60 (81%)	27 (36%)	0.27

The overall RNA backbone suiteness is 0.08.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	2	C	12
2	B	3	G	12
2	B	4	G	12
2	B	5	A	12
2	B	7	U	12

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	4	G	12

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Mol	Chain	Res	Type	Models (Total)
2	B	3	G	7
2	B	2	C	6
2	B	1	U	2

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 58% for the well-defined parts and 53% 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	1436
Number of shifts mapped to atoms	1436
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	-0.29 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	133	0.14 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient 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 58%, i.e. 1269 atoms were assigned a chemical shift out of a possible 2195. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	343/732 (47%)	238/298 (80%)	105/294 (36%)	0/140 (0%)
Sidechain	902/1214 (74%)	635/791 (80%)	267/369 (72%)	0/54 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	24/118 (20%)	24/58 (41%)	0/50 (0%)	0/10 (0%)
Sugar	0/77 (0%)	0/42 (0%)	0/35 (0%)	0/0 (—%)
Base	0/54 (0%)	0/33 (0%)	0/12 (0%)	0/9 (0%)
Overall	1269/2195 (58%)	897/1222 (73%)	372/760 (49%)	0/213 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 1436 atoms were assigned a chemical shift out of a possible 2687. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	390/944 (41%)	271/385 (70%)	119/382 (31%)	0/177 (0%)
Sidechain	1018/1474 (69%)	717/959 (75%)	301/455 (66%)	0/60 (0%)
Aromatic	28/138 (20%)	28/68 (41%)	0/60 (0%)	0/10 (0%)
Sugar	0/77 (0%)	0/42 (0%)	0/35 (0%)	0/0 (—%)
Base	0/54 (0%)	0/33 (0%)	0/12 (0%)	0/9 (0%)
Overall	1436/2687 (53%)	1016/1487 (68%)	420/944 (44%)	0/256 (0%)

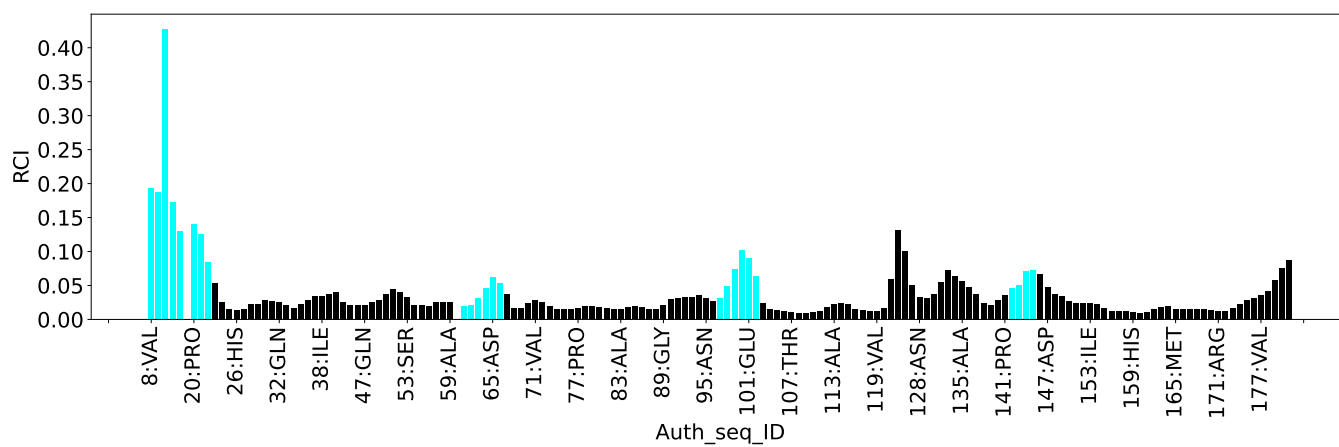
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2220
Intra-residue ($ i-j =0$)	1208
Sequential ($ i-j =1$)	430
Medium range ($ i-j >1$ and $ i-j <5$)	172
Long range ($ i-j \geq 5$)	355
Inter-chain	37
Hydrogen bond restraints	18
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.2
Number of long range restraints per residue ¹	1.8

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)	33.5	0.2
0.2-0.5 (Medium)	45.4	0.5
>0.5 (Large)	54.3	7.18

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 ⓘ

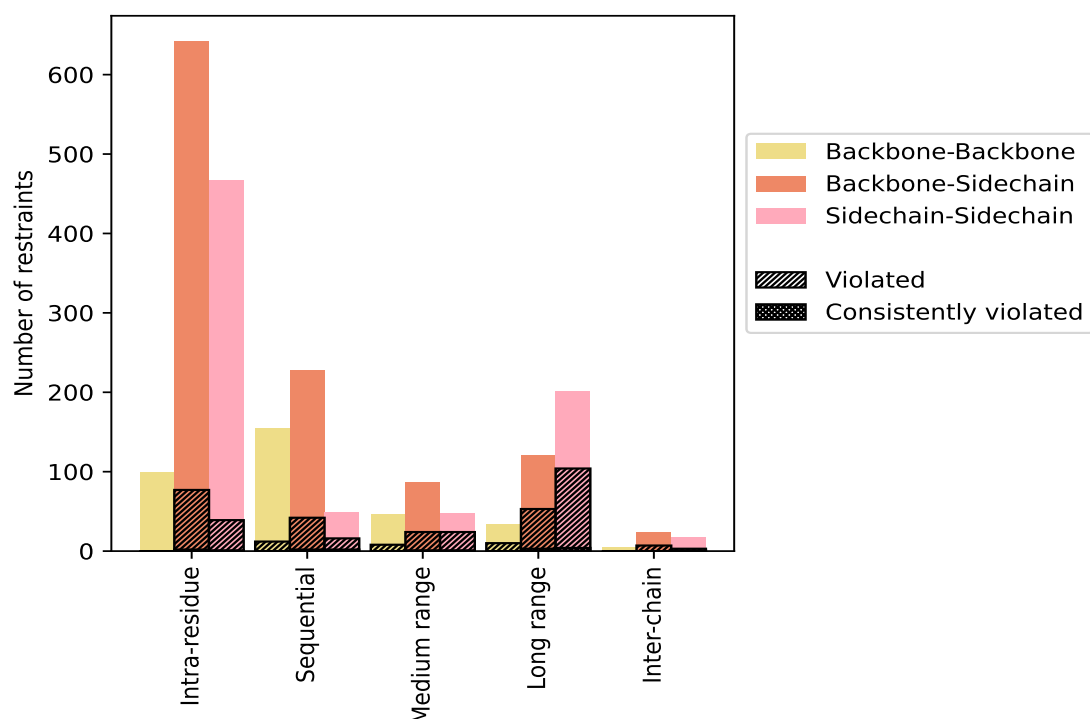
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1208	54.4	116	9.6	5.2	3	0.2	0.1
Backbone-Backbone	99	4.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	642	28.9	77	12.0	3.5	2	0.3	0.1
Sidechain-Sidechain	467	21.0	39	8.4	1.8	1	0.2	0.0
Sequential ($i-j =1$)	430	19.4	70	16.3	3.2	4	0.9	0.2
Backbone-Backbone	155	7.0	12	7.7	0.5	0	0.0	0.0
Backbone-Sidechain	228	10.3	42	18.4	1.9	2	0.9	0.1
Sidechain-Sidechain	47	2.1	16	34.0	0.7	2	4.3	0.1
Medium range ($i-j >1$ & $i-j <5$)	172	7.7	56	32.6	2.5	2	1.2	0.1
Backbone-Backbone	46	2.1	8	17.4	0.4	0	0.0	0.0
Backbone-Sidechain	79	3.6	24	30.4	1.1	1	1.3	0.0
Sidechain-Sidechain	47	2.1	24	51.1	1.1	1	2.1	0.0
Long range ($i-j \geq 5$)	355	16.0	167	47.0	7.5	7	2.0	0.3
Backbone-Backbone	33	1.5	10	30.3	0.5	0	0.0	0.0
Backbone-Sidechain	121	5.5	53	43.8	2.4	3	2.5	0.1
Sidechain-Sidechain	201	9.1	104	51.7	4.7	4	2.0	0.2
Inter-chain	37	1.7	10	27.0	0.5	1	2.7	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	19	0.9	7	36.8	0.3	0	0.0	0.0
Sidechain-Sidechain	13	0.6	3	23.1	0.1	1	7.7	0.0
Hydrogen bond	18	0.8	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	2220	100.0	419	18.9	18.9	17	0.8	0.8
Backbone-Backbone	338	15.2	30	8.9	1.4	0	0.0	0.0
Backbone-Sidechain	1101	49.6	203	18.4	9.1	8	0.7	0.4
Sidechain-Sidechain	781	35.2	186	23.8	8.4	9	1.2	0.4

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	29	20	24	64	2	139	0.65	4.93	0.75	0.38
2	33	18	25	53	2	131	0.7	4.87	0.78	0.41
3	42	24	21	70	3	160	0.65	4.7	0.78	0.38
4	26	16	20	55	2	119	0.71	5.8	0.94	0.36
5	39	22	30	63	1	155	0.69	7.18	0.97	0.37
6	36	19	22	64	4	145	0.82	5.73	0.93	0.47
7	31	19	17	42	3	112	0.67	5.69	0.87	0.35
8	33	22	24	53	5	137	0.66	6.56	0.88	0.4
9	41	19	23	57	1	141	0.74	6.89	1.03	0.43
10	35	18	21	55	4	133	0.83	6.9	1.09	0.39

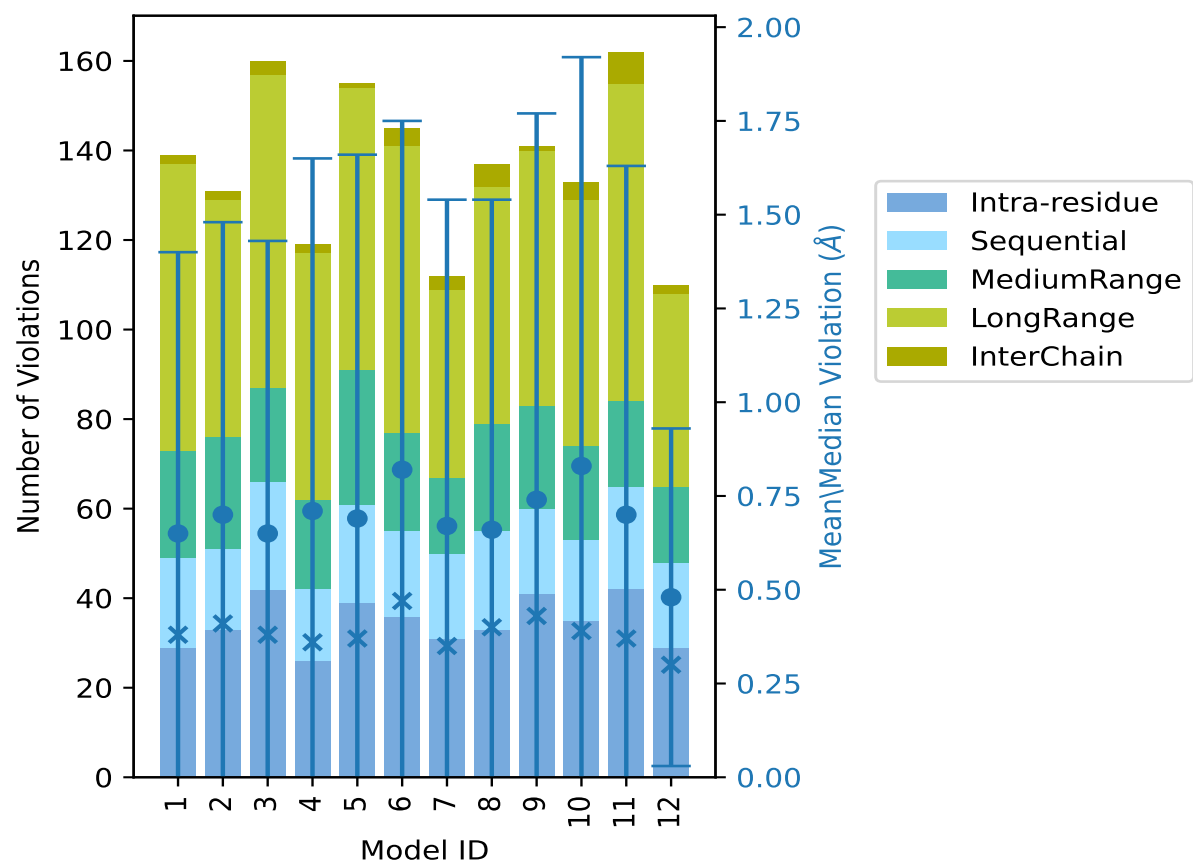
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	42	23	19	71	7	162	0.7	7.02	0.93	0.37
12	29	19	17	43	2	110	0.48	2.37	0.45	0.3

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

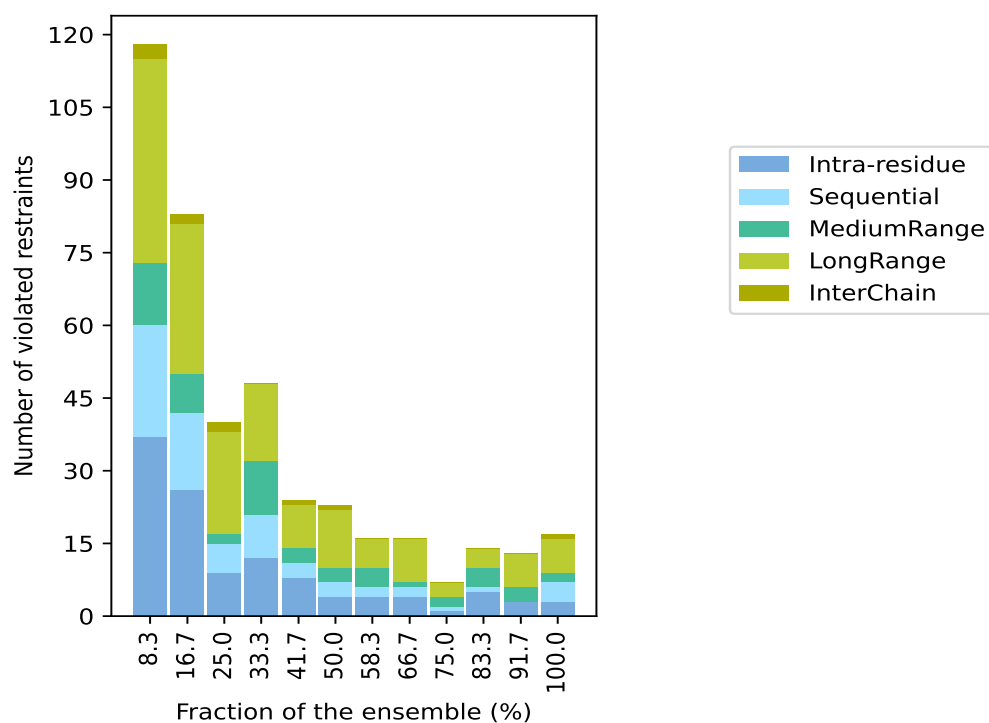
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1783(IR:1092, SQ:360, MR:116, LR:188, IC:27) restraints are 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	%
37	23	13	42	3	118	1	8.3
26	16	8	31	2	83	2	16.7
9	6	2	21	2	40	3	25.0
12	9	11	16	0	48	4	33.3
8	3	3	9	1	24	5	41.7
4	3	3	12	1	23	6	50.0
4	2	4	6	0	16	7	58.3
4	2	1	9	0	16	8	66.7
1	1	2	3	0	7	9	75.0
5	1	4	4	0	14	10	83.3
3	0	3	7	0	13	11	91.7
3	4	2	7	1	17	12	100.0

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

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

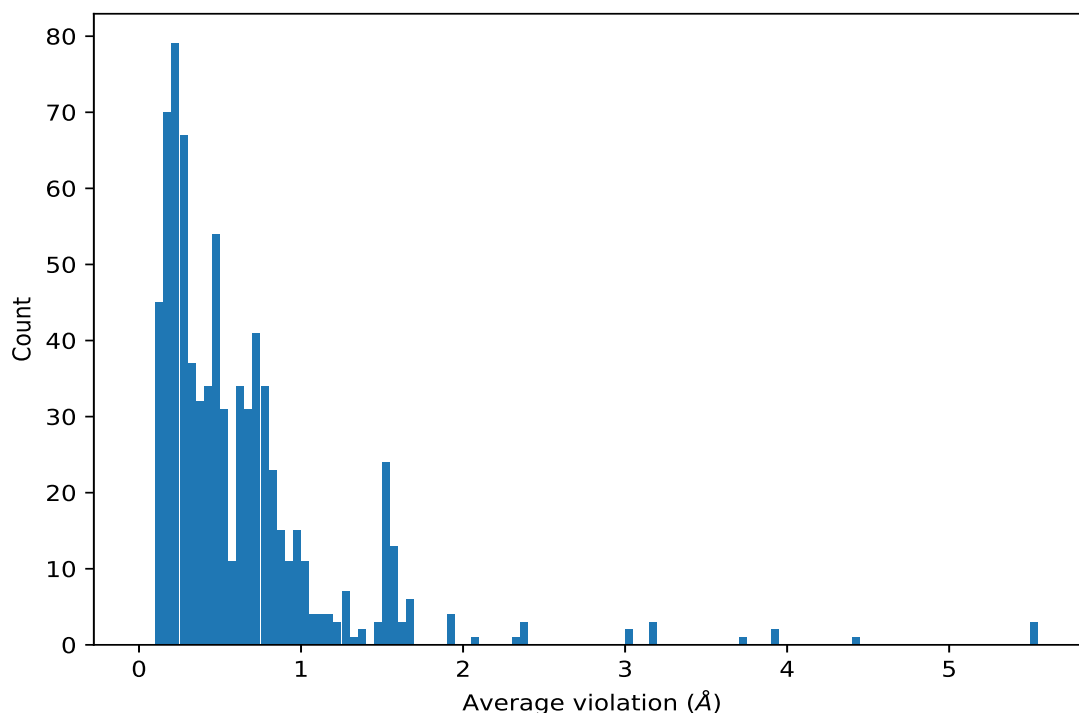
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	12	3.72	1.54	3.69
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	12	3.18	1.16	3.08
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	12	3.18	1.16	3.08
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	12	3.18	1.16	3.08
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	12	1.56	1.64	0.41
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	12	1.56	1.64	0.41
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	12	1.56	1.64	0.41
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG2	12	1.56	1.64	0.41
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG2	12	1.56	1.64	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG2	12	1.56	1.64	0.41
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	12	1.46	0.33	1.49
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	12	1.46	0.33	1.49
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	12	1.46	0.33	1.49
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	12	1.26	0.65	0.97
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	12	1.18	0.21	1.17
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	12	1.14	0.32	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	12	1.14	0.32	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	12	1.14	0.32	1.27
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	12	0.93	0.36	0.91
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	12	0.93	0.36	0.91
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	12	0.93	0.36	0.91
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	12	0.83	0.24	0.88
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	12	0.83	0.24	0.88
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	12	0.83	0.24	0.88
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	12	0.82	0.54	0.68
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	12	0.82	0.54	0.68
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	12	0.82	0.54	0.68
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	12	0.7	0.41	0.59
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	12	0.7	0.41	0.59
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	12	0.7	0.41	0.59
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	12	0.52	0.4	0.49
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	12	0.52	0.4	0.49
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	12	0.49	0.09	0.5
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	12	0.49	0.09	0.5
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	12	0.49	0.09	0.5
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	12	0.4	0.13	0.34
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	12	0.34	0.1	0.34
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB3	12	0.34	0.1	0.34
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	12	0.22	0.04	0.22
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD3	12	0.22	0.04	0.22
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	12	0.17	0.02	0.16
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	11	4.42	0.86	4.65
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	11	2.07	1.08	2.03
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	11	1.65	1.15	1.83
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	11	1.65	1.15	1.83
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	11	1.65	1.15	1.83
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	11	1.37	0.21	1.46
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	11	1.18	0.68	1.25
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	11	1.18	0.68	1.25
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	11	1.18	0.68	1.25
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	11	0.89	0.12	0.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	11	0.89	0.12	0.91
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	11	0.89	0.12	0.91
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	11	0.83	0.38	0.66
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	11	0.8	0.36	0.75
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	11	0.8	0.75	0.37
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	11	0.75	0.32	0.79
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	11	0.75	0.32	0.79
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	11	0.75	0.32	0.79
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	11	0.61	0.05	0.63
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	11	0.18	0.02	0.17
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	11	0.16	0.02	0.16
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD3	11	0.16	0.02	0.16
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	10	5.51	1.5	5.8
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	10	5.51	1.5	5.8
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	10	5.51	1.5	5.8
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	10	1.94	0.24	1.94
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	10	0.98	0.8	0.79
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	10	0.98	0.8	0.79
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	10	0.98	0.8	0.79
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD2	10	0.98	0.8	0.79
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD2	10	0.98	0.8	0.79
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD2	10	0.98	0.8	0.79
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	10	0.92	0.43	1.02
(1,1686)	1:113:A:ALA:HB3	1:150:A:GLU:HB3	10	0.92	0.43	1.02
(1,1686)	1:113:A:ALA:HB2	1:150:A:GLU:HB3	10	0.92	0.43	1.02
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	10	0.79	0.68	0.41
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	10	0.79	0.68	0.41
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	10	0.79	0.68	0.41
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG2	10	0.79	0.68	0.41
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG2	10	0.79	0.68	0.41
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG2	10	0.79	0.68	0.41
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	10	0.7	0.26	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	10	0.7	0.26	0.66
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	10	0.48	0.24	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	10	0.48	0.24	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	10	0.48	0.24	0.42
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	10	0.44	0.01	0.44
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	10	0.39	0.19	0.43
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	10	0.28	0.02	0.27
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	10	0.26	0.04	0.26
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	10	0.26	0.04	0.26
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	10	0.19	0.05	0.2
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	10	0.13	0.02	0.12
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	10	0.11	0.01	0.11
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	9	0.84	0.24	0.93
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	9	0.84	0.24	0.93
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	9	0.84	0.24	0.93
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	9	0.71	0.58	0.31
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	9	0.71	0.58	0.31
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	9	0.71	0.58	0.31
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	9	0.7	0.48	0.62
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG11	9	0.6	0.36	0.49
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG12	9	0.6	0.36	0.49
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG13	9	0.6	0.36	0.49
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	9	0.6	0.36	0.49
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	9	0.6	0.36	0.49
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	9	0.6	0.36	0.49
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	9	0.36	0.16	0.33
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	9	0.36	0.16	0.33
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	9	0.36	0.16	0.33
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	9	0.27	0.21	0.21
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	9	0.21	0.06	0.23
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	8	1.62	0.66	1.96
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	8	1.62	0.66	1.96
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	8	1.62	0.66	1.96
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	8	0.8	0.51	0.59
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	8	0.8	0.51	0.59
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	8	0.8	0.51	0.59
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	8	0.78	0.29	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	8	0.78	0.29	0.7
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	8	0.78	0.29	0.7
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	8	0.74	0.34	0.65
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	8	0.74	0.34	0.65
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	8	0.74	0.34	0.65
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	8	0.53	0.25	0.56
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	8	0.53	0.25	0.56
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	8	0.53	0.25	0.56
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	8	0.38	0.01	0.38
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	8	0.38	0.01	0.38
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	8	0.38	0.01	0.38
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	8	0.38	0.22	0.3
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	8	0.38	0.22	0.3
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	8	0.38	0.22	0.3
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG21	8	0.34	0.16	0.35
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG22	8	0.34	0.16	0.35
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG23	8	0.34	0.16	0.35
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	8	0.34	0.16	0.35
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	8	0.34	0.16	0.35
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	8	0.34	0.16	0.35
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	8	0.33	0.11	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	8	0.33	0.11	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	8	0.33	0.11	0.29
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	8	0.28	0.19	0.2
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	8	0.28	0.19	0.2
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	8	0.28	0.19	0.2
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	8	0.28	0.12	0.3
(1,1756)	1:57:A:LYS:HE3	1:57:A:LYS:HB2	8	0.28	0.12	0.3
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	8	0.25	0.05	0.25
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	8	0.25	0.05	0.25
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	8	0.22	0.11	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG2	8	0.22	0.11	0.19
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	8	0.19	0.09	0.17
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	8	0.19	0.06	0.2
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	8	0.11	0.01	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	8	0.11	0.01	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	8	0.11	0.01	0.11
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	7	2.36	0.98	2.68
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	7	2.36	0.98	2.68
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	7	2.36	0.98	2.68
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	7	1.58	0.33	1.69
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	7	1.58	0.33	1.69
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	7	1.58	0.33	1.69
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD11	7	1.58	0.33	1.69
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD12	7	1.58	0.33	1.69
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD13	7	1.58	0.33	1.69
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	7	0.81	0.36	0.8
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	7	0.81	0.36	0.8
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	7	0.68	0.3	0.65
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	7	0.68	0.3	0.65
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	7	0.68	0.3	0.65
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	7	0.64	0.49	0.43
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	7	0.64	0.49	0.43
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	7	0.64	0.49	0.43
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	7	0.6	0.3	0.58
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	7	0.6	0.3	0.58
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	7	0.56	0.4	0.37
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD3	7	0.52	0.06	0.5
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD2	7	0.52	0.06	0.5
(1,1299)	1:102:A:GLU:HG3	1:102:A:GLU:H	7	0.43	0.12	0.47
(1,1299)	1:102:A:GLU:HG2	1:102:A:GLU:H	7	0.43	0.12	0.47
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	7	0.4	0.05	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	7	0.4	0.05	0.4
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	7	0.24	0.05	0.23
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	7	0.24	0.05	0.23
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	7	0.22	0.11	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	7	0.22	0.11	0.14
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	7	0.22	0.11	0.14
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	7	0.2	0.07	0.17
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	7	0.2	0.07	0.17
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	7	0.2	0.07	0.17
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	7	0.18	0.08	0.14
(1,1123)	1:86:A:ARG:HD2	1:86:A:ARG:HG2	7	0.18	0.08	0.14
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	7	0.16	0.04	0.14
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG2	7	0.16	0.04	0.14
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	7	0.15	0.03	0.16
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	6	1.9	1.09	1.72
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	6	1.9	1.09	1.72
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	6	1.9	1.09	1.72
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	6	1.52	0.85	1.3
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	6	1.52	0.85	1.3
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	6	1.52	0.85	1.3
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	6	1.36	0.14	1.33
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	6	0.98	0.64	0.98
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	6	0.98	0.64	0.98
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	6	0.98	0.64	0.98
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	6	0.85	0.73	0.73
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	6	0.85	0.73	0.73
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	6	0.85	0.73	0.73
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	6	0.83	0.41	0.66
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG3	6	0.78	0.89	0.38
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG3	6	0.78	0.89	0.38
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG2	6	0.78	0.89	0.38
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG2	6	0.78	0.89	0.38
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	6	0.75	0.11	0.76
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	6	0.75	0.11	0.76
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	6	0.75	0.11	0.76
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	6	0.7	0.48	0.63
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	6	0.67	0.28	0.76
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	6	0.67	0.28	0.76
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	6	0.67	0.28	0.76
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	6	0.67	0.28	0.76
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	6	0.67	0.28	0.76
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	6	0.67	0.28	0.76
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	6	0.59	0.44	0.44
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	6	0.59	0.44	0.44
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	6	0.59	0.44	0.44
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	6	0.55	0.08	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	6	0.55	0.08	0.57
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	6	0.55	0.08	0.57
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	6	0.5	0.33	0.47
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	6	0.5	0.33	0.47
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	6	0.5	0.33	0.47
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG21	6	0.49	0.48	0.25
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG22	6	0.49	0.48	0.25
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG23	6	0.49	0.48	0.25
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG21	6	0.49	0.48	0.25
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG22	6	0.49	0.48	0.25
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG23	6	0.49	0.48	0.25
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	6	0.49	0.01	0.48
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	6	0.49	0.01	0.48
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	6	0.49	0.01	0.48
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	6	0.24	0.14	0.21
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	6	0.24	0.1	0.21
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	6	0.24	0.07	0.26
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	6	0.24	0.07	0.26
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	6	0.24	0.07	0.26
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB3	6	0.24	0.07	0.26
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB3	6	0.24	0.07	0.26
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB3	6	0.24	0.07	0.26
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	6	0.21	0.09	0.18
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	6	0.21	0.09	0.18
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	6	0.21	0.09	0.18
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	6	0.2	0.18	0.12
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	6	0.16	0.03	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	6	0.16	0.03	0.16
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	6	0.12	0.0	0.12
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	6	0.11	0.01	0.11
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	6	0.11	0.01	0.11
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	6	0.11	0.01	0.11
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	5	3.94	1.71	4.84
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	5	3.94	1.71	4.84
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	5	2.33	1.15	2.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	5	1.54	0.79	1.24
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	5	1.54	0.79	1.24
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	5	1.54	0.79	1.24
(1,1782)	1:92:A:LYS:HE2	1:92:A:LYS:HB3	5	1.0	0.43	1.22
(1,1782)	1:92:A:LYS:HE3	1:92:A:LYS:HB3	5	1.0	0.43	1.22
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD2	5	0.89	0.4	1.08
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD2	5	0.89	0.4	1.08
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD2	5	0.89	0.4	1.08
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD3	5	0.89	0.4	1.08
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD3	5	0.89	0.4	1.08
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD3	5	0.89	0.4	1.08
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	5	0.84	0.43	0.96
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	5	0.84	0.43	0.96
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG3	5	0.74	0.23	0.58
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG2	5	0.74	0.23	0.58
(1,1622)	1:92:A:LYS:HE3	1:92:A:LYS:HG3	5	0.74	0.23	0.58
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD2	5	0.52	0.12	0.54
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD3	5	0.52	0.12	0.54
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	5	0.52	0.17	0.47
(1,1022)	1:141:A:PRO:HD2	1:141:A:PRO:HB3	5	0.5	0.02	0.5
(1,1022)	1:141:A:PRO:HD3	1:141:A:PRO:HB3	5	0.5	0.02	0.5
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	5	0.5	0.2	0.57
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	5	0.49	0.2	0.58
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	5	0.49	0.18	0.51
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	5	0.49	0.18	0.51
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	5	0.49	0.18	0.51
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	5	0.45	0.19	0.38
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	5	0.42	0.21	0.37
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	5	0.42	0.21	0.37
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	5	0.42	0.21	0.37
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	5	0.39	0.15	0.43
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	5	0.39	0.15	0.43
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	5	0.39	0.15	0.43
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	5	0.36	0.14	0.32
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	5	0.31	0.11	0.33
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB2	5	0.3	0.02	0.31
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB3	5	0.3	0.02	0.31
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	5	0.29	0.12	0.29
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	5	0.29	0.12	0.29
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	5	0.29	0.12	0.29
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	5	0.22	0.09	0.22
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	5	0.22	0.09	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	5	0.22	0.09	0.22
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	5	0.17	0.08	0.11
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	5	0.12	0.02	0.13
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	5	0.12	0.01	0.11
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD1	4	3.0	1.33	3.56
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD2	4	3.0	1.33	3.56
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG2	4	1.69	0.18	1.64
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG3	4	1.69	0.18	1.64
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD21	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD22	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD23	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD21	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD22	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD23	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD21	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD22	4	1.5	0.46	1.6
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD23	4	1.5	0.46	1.6
(1,1901)	1:153:A:ILE:HB	1:110:A:ARG:HD2	4	1.22	0.23	1.31
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG3	4	1.2	0.91	1.25
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG2	4	1.2	0.91	1.25
(2,81)	1:140:A:VAL:HG11	1:119:A:VAL:HA	4	1.07	0.41	1.2
(2,81)	1:140:A:VAL:HG12	1:119:A:VAL:HA	4	1.07	0.41	1.2
(2,81)	1:140:A:VAL:HG13	1:119:A:VAL:HA	4	1.07	0.41	1.2
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE1	4	1.0	0.79	0.66
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE2	4	1.0	0.79	0.66
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE1	4	1.0	0.79	0.66
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE2	4	1.0	0.79	0.66
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE1	4	1.0	0.79	0.66
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE2	4	1.0	0.79	0.66
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG21	4	0.97	0.24	1.02
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG22	4	0.97	0.24	1.02
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG23	4	0.97	0.24	1.02
(1,987)	1:63:A:THR:HG21	1:62:A:GLU:HB3	4	0.92	0.18	0.84
(1,987)	1:63:A:THR:HG22	1:62:A:GLU:HB3	4	0.92	0.18	0.84
(1,987)	1:63:A:THR:HG23	1:62:A:GLU:HB3	4	0.92	0.18	0.84
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD1	4	0.92	0.06	0.92
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD2	4	0.92	0.06	0.92
(1,1269)	1:58:A:ILE:HG12	1:58:A:ILE:H	4	0.86	0.12	0.85
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD21	4	0.77	0.59	0.54
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD22	4	0.77	0.59	0.54
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD23	4	0.77	0.59	0.54
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD21	4	0.77	0.59	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD22	4	0.77	0.59	0.54
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD23	4	0.77	0.59	0.54
(1,1309)	1:91:A:LEU:HD21	1:96:A:PHE:HB2	4	0.74	0.54	0.6
(1,1309)	1:91:A:LEU:HD22	1:96:A:PHE:HB2	4	0.74	0.54	0.6
(1,1309)	1:91:A:LEU:HD23	1:96:A:PHE:HB2	4	0.74	0.54	0.6
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD1	4	0.7	0.35	0.84
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD2	4	0.7	0.35	0.84
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD1	4	0.7	0.35	0.84
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD2	4	0.7	0.35	0.84
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD1	4	0.7	0.35	0.84
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD2	4	0.7	0.35	0.84
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD11	4	0.7	0.39	0.73
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD12	4	0.7	0.39	0.73
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD13	4	0.7	0.39	0.73
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD11	4	0.7	0.39	0.73
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD12	4	0.7	0.39	0.73
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD13	4	0.7	0.39	0.73
(1,1119)	1:91:A:LEU:HD21	1:91:A:LEU:HA	4	0.69	0.06	0.7
(1,1119)	1:91:A:LEU:HD22	1:91:A:LEU:HA	4	0.69	0.06	0.7
(1,1119)	1:91:A:LEU:HD23	1:91:A:LEU:HA	4	0.69	0.06	0.7
(1,700)	1:128:A:ASN:HB3	1:125:A:LYS:HA	4	0.67	0.1	0.72
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG11	4	0.62	0.11	0.61
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG12	4	0.62	0.11	0.61
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG13	4	0.62	0.11	0.61
(1,489)	1:172:A:ASP:H	1:171:A:ARG:HG3	4	0.55	0.03	0.56
(1,1275)	1:92:A:LYS:HD2	1:92:A:LYS:HA	4	0.53	0.26	0.46
(1,1490)	1:115:A:ALA:HB1	1:112:A:PRO:HD2	4	0.52	0.08	0.52
(1,1490)	1:115:A:ALA:HB2	1:112:A:PRO:HD2	4	0.52	0.08	0.52
(1,1490)	1:115:A:ALA:HB3	1:112:A:PRO:HD2	4	0.52	0.08	0.52
(1,1378)	1:142:A:ARG:HB2	1:141:A:PRO:HB3	4	0.5	0.22	0.5
(1,1378)	1:142:A:ARG:HB3	1:141:A:PRO:HB3	4	0.5	0.22	0.5
(1,1220)	1:146:A:PRO:HD2	1:144:A:GLN:HG2	4	0.49	0.35	0.4
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG21	4	0.48	0.21	0.55
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG22	4	0.48	0.21	0.55
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG23	4	0.48	0.21	0.55
(1,1691)	1:110:A:ARG:HD2	1:151:A:GLN:HB2	4	0.46	0.12	0.43
(1,1783)	1:116:A:ALA:HB1	1:140:A:VAL:HB	4	0.45	0.21	0.4
(1,1783)	1:116:A:ALA:HB2	1:140:A:VAL:HB	4	0.45	0.21	0.4
(1,1783)	1:116:A:ALA:HB3	1:140:A:VAL:HB	4	0.45	0.21	0.4
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG11	4	0.44	0.02	0.44
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG12	4	0.44	0.02	0.44
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG13	4	0.44	0.02	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,539)	1:179:A:GLN:H	1:176:A:GLN:HA	4	0.36	0.05	0.34
(1,1496)	1:87:A:ILE:HB	1:84:A:GLN:HA	4	0.36	0.13	0.32
(1,1469)	1:32:A:GLN:HG3	1:32:A:GLN:HA	4	0.35	0.07	0.38
(1,483)	1:143:A:ASP:H	1:142:A:ARG:HG2	4	0.34	0.09	0.36
(1,1663)	1:105:A:LEU:HD11	1:88:A:TYR:HA	4	0.32	0.12	0.3
(1,1663)	1:105:A:LEU:HD12	1:88:A:TYR:HA	4	0.32	0.12	0.3
(1,1663)	1:105:A:LEU:HD13	1:88:A:TYR:HA	4	0.32	0.12	0.3
(1,693)	1:126:A:THR:HB	1:126:A:THR:HA	4	0.32	0.0	0.32
(1,1717)	1:50:A:ARG:HD3	1:50:A:ARG:HB2	4	0.31	0.07	0.32
(1,1717)	1:50:A:ARG:HD2	1:50:A:ARG:HB3	4	0.31	0.07	0.32
(1,830)	1:171:A:ARG:HA	1:174:A:LEU:HB3	4	0.26	0.11	0.22
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG21	4	0.24	0.01	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG22	4	0.24	0.01	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG23	4	0.24	0.01	0.24
(1,1412)	1:171:A:ARG:HB3	1:168:A:ARG:HA	4	0.24	0.1	0.24
(1,1668)	1:32:A:GLN:HA	1:32:A:GLN:HB2	4	0.22	0.01	0.22
(1,1443)	1:58:A:ILE:HG21	1:58:A:ILE:HA	4	0.22	0.04	0.23
(1,1443)	1:58:A:ILE:HG22	1:58:A:ILE:HA	4	0.22	0.04	0.23
(1,1443)	1:58:A:ILE:HG23	1:58:A:ILE:HA	4	0.22	0.04	0.23
(1,1654)	1:105:A:LEU:HD21	1:91:A:LEU:HG	4	0.22	0.06	0.22
(1,1654)	1:105:A:LEU:HD22	1:91:A:LEU:HG	4	0.22	0.06	0.22
(1,1654)	1:105:A:LEU:HD23	1:91:A:LEU:HG	4	0.22	0.06	0.22
(1,221)	1:91:A:LEU:H	1:91:A:LEU:HG	4	0.2	0.09	0.18
(1,218)	1:96:A:PHE:H	1:94:A:GLU:HB2	4	0.19	0.06	0.18
(2,53)	1:58:A:ILE:HD11	1:71:A:VAL:HA	4	0.17	0.08	0.14
(2,53)	1:58:A:ILE:HD12	1:71:A:VAL:HA	4	0.17	0.08	0.14
(2,53)	1:58:A:ILE:HD13	1:71:A:VAL:HA	4	0.17	0.08	0.14
(1,452)	1:98:A:GLY:H	1:99:A:PRO:HB2	4	0.17	0.06	0.16
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB1	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB2	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB3	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB1	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB2	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB3	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB1	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB2	4	0.15	0.01	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB3	4	0.15	0.01	0.15
(1,2088)	1:171:A:ARG:H	1:172:A:ASP:H	4	0.14	0.02	0.14
(1,1326)	1:118:A:ARG:HB3	1:118:A:ARG:HG2	4	0.11	0.0	0.11
(1,1326)	1:118:A:ARG:HB2	1:118:A:ARG:HG2	4	0.11	0.0	0.11
(1,1326)	1:118:A:ARG:HB2	1:118:A:ARG:HG3	4	0.11	0.0	0.11
(1,2094)	1:177:A:VAL:H	1:178:A:LYS:H	4	0.1	0.0	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,428)	1:150:A:GLU:H	1:151:A:GLN:HG3	3	1.34	0.26	1.31
(2,101)	1:143:A:ASP:OD2	2:4:B:G:H21	3	1.1	0.2	1.16
(1,2023)	1:118:A:ARG:HD3	2:2:B:C:H2'	3	1.08	0.7	1.42
(1,1742)	1:91:A:LEU:HD21	1:30:A:PRO:HD2	3	1.04	0.49	1.08
(1,1742)	1:91:A:LEU:HD22	1:30:A:PRO:HD2	3	1.04	0.49	1.08
(1,1742)	1:91:A:LEU:HD23	1:30:A:PRO:HD2	3	1.04	0.49	1.08
(1,993)	1:154:A:VAL:HG11	1:153:A:ILE:HA	3	0.99	0.01	0.99
(1,993)	1:154:A:VAL:HG12	1:153:A:ILE:HA	3	0.99	0.01	0.99
(1,993)	1:154:A:VAL:HG13	1:153:A:ILE:HA	3	0.99	0.01	0.99
(1,1320)	1:131:A:GLN:HG3	1:135:A:ALA:HA	3	0.89	0.24	0.73
(2,64)	1:53:A:SER:HB2	1:82:A:LYS:HD2	3	0.87	0.25	0.84
(1,975)	1:57:A:LYS:HB2	1:72:A:VAL:HB	3	0.8	0.16	0.85
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG21	3	0.67	0.09	0.72
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG22	3	0.67	0.09	0.72
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG23	3	0.67	0.09	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG21	3	0.67	0.09	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG22	3	0.67	0.09	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG23	3	0.67	0.09	0.72
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG21	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG22	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG23	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG21	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG22	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG23	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG21	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG22	3	0.66	0.11	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG23	3	0.66	0.11	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG21	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG22	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG23	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG21	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG22	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG23	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG21	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG22	3	0.64	0.02	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG23	3	0.64	0.02	0.64
(1,762)	1:178:A:LYS:HA	1:181:A:HIS:HB3	3	0.55	0.11	0.53
(1,454)	1:165:A:MET:H	1:164:A:GLN:HG2	3	0.54	0.14	0.55
(1,988)	1:32:A:GLN:HG3	1:32:A:GLN:HB2	3	0.5	0.02	0.51
(1,1118)	1:91:A:LEU:HD21	1:30:A:PRO:HD3	3	0.48	0.29	0.53
(1,1118)	1:91:A:LEU:HD22	1:30:A:PRO:HD3	3	0.48	0.29	0.53
(1,1118)	1:91:A:LEU:HD23	1:30:A:PRO:HD3	3	0.48	0.29	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB1	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB2	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB3	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB1	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB2	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB3	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB1	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB2	3	0.41	0.1	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB3	3	0.41	0.1	0.37
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG21	3	0.41	0.08	0.45
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG22	3	0.41	0.08	0.45
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG23	3	0.41	0.08	0.45
(1,1939)	1:28:A:PHE:HD1	1:106:A:GLU:HG2	3	0.38	0.03	0.38
(1,1939)	1:28:A:PHE:HD2	1:106:A:GLU:HG2	3	0.38	0.03	0.38
(1,1563)	1:100:A:LYS:HA	1:100:A:LYS:HD3	3	0.35	0.23	0.19
(1,1563)	1:100:A:LYS:HA	1:100:A:LYS:HD2	3	0.35	0.23	0.19
(1,1791)	1:104:A:LYS:HE3	1:104:A:LYS:HB3	3	0.31	0.15	0.22
(1,1791)	1:104:A:LYS:HE2	1:104:A:LYS:HB3	3	0.31	0.15	0.22
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD11	3	0.31	0.14	0.37
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD12	3	0.31	0.14	0.37
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD13	3	0.31	0.14	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD11	3	0.31	0.14	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD12	3	0.31	0.14	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD13	3	0.31	0.14	0.37
(1,1708)	1:48:A:LEU:HD11	1:48:A:LEU:HB2	3	0.29	0.02	0.29
(1,1708)	1:48:A:LEU:HD12	1:48:A:LEU:HB2	3	0.29	0.02	0.29
(1,1708)	1:48:A:LEU:HD13	1:48:A:LEU:HB2	3	0.29	0.02	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG11	3	0.29	0.12	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG12	3	0.29	0.12	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG13	3	0.29	0.12	0.29
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG11	3	0.29	0.12	0.29
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG12	3	0.29	0.12	0.29
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG13	3	0.29	0.12	0.29
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG21	3	0.28	0.07	0.32
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG22	3	0.28	0.07	0.32
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG23	3	0.28	0.07	0.32
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG21	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG22	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG23	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG21	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG22	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG23	3	0.28	0.09	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG21	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG22	3	0.28	0.09	0.23
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG23	3	0.28	0.09	0.23
(1,1840)	1:27:A:VAL:HG11	1:107:A:THR:HA	3	0.25	0.05	0.26
(1,1840)	1:27:A:VAL:HG12	1:107:A:THR:HA	3	0.25	0.05	0.26
(1,1840)	1:27:A:VAL:HG13	1:107:A:THR:HA	3	0.25	0.05	0.26
(1,1466)	1:131:A:GLN:HG3	1:131:A:GLN:HA	3	0.25	0.1	0.3
(1,1621)	1:151:A:GLN:HA	1:112:A:PRO:HA	3	0.24	0.07	0.26
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD11	3	0.23	0.06	0.21
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD12	3	0.23	0.06	0.21
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD13	3	0.23	0.06	0.21
(1,1948)	1:96:A:PHE:HD1	1:91:A:LEU:HA	3	0.23	0.12	0.15
(1,1948)	1:96:A:PHE:HD2	1:91:A:LEU:HA	3	0.23	0.12	0.15
(1,1722)	1:76:A:PRO:HB2	1:77:A:PRO:HG2	3	0.21	0.11	0.17
(1,1520)	1:179:A:GLN:HA	1:179:A:GLN:HG3	3	0.2	0.1	0.17
(1,1912)	1:156:A:ILE:HG21	1:166:A:ALA:HA	3	0.2	0.06	0.19
(1,1912)	1:156:A:ILE:HG22	1:166:A:ALA:HA	3	0.2	0.06	0.19
(1,1912)	1:156:A:ILE:HG23	1:166:A:ALA:HA	3	0.2	0.06	0.19
(1,1716)	1:67:A:LYS:HG3	1:67:A:LYS:HA	3	0.19	0.01	0.2
(1,1445)	1:146:A:PRO:HD3	1:145:A:THR:HA	3	0.19	0.05	0.2
(1,1851)	1:153:A:ILE:HG21	1:141:A:PRO:HD3	3	0.18	0.06	0.2
(1,1851)	1:153:A:ILE:HG22	1:141:A:PRO:HD3	3	0.18	0.06	0.2
(1,1851)	1:153:A:ILE:HG23	1:141:A:PRO:HD3	3	0.18	0.06	0.2
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG21	3	0.17	0.01	0.17
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG22	3	0.17	0.01	0.17
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG23	3	0.17	0.01	0.17
(1,1587)	1:104:A:LYS:HE2	1:104:A:LYS:HG2	3	0.15	0.04	0.18
(1,333)	1:32:A:GLN:H	1:32:A:GLN:HB3	3	0.12	0.0	0.12
(1,2082)	1:165:A:MET:H	1:166:A:ALA:H	3	0.12	0.03	0.11
(2,21)	1:63:A:THR:H	1:66:A:SER:HB2	2	1.69	0.99	1.69
(1,2065)	1:73:A:ILE:HA	1:56:A:ILE:HA	2	1.58	0.12	1.58
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG21	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG22	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG23	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG21	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG22	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG23	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG21	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG22	2	1.51	0.62	1.51
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG23	2	1.51	0.62	1.51
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB1	2	1.28	0.91	1.28
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB2	2	1.28	0.91	1.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB3	2	1.28	0.91	1.28
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB1	2	1.28	0.91	1.28
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB2	2	1.28	0.91	1.28
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB3	2	1.28	0.91	1.28
(1,1873)	1:178:A:LYS:HE2	1:178:A:LYS:HB3	2	0.84	0.02	0.84
(1,107)	1:178:A:LYS:H	1:177:A:VAL:HB	2	0.82	0.05	0.82
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG11	2	0.75	0.17	0.75
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG12	2	0.75	0.17	0.75
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG13	2	0.75	0.17	0.75
(1,1632)	1:178:A:LYS:HE3	1:178:A:LYS:HG2	2	0.72	0.02	0.72
(1,1632)	1:178:A:LYS:HE2	1:178:A:LYS:HG2	2	0.72	0.02	0.72
(2,69)	1:93:A:GLU:HB3	1:94:A:GLU:HB2	2	0.72	0.53	0.72
(1,1128)	1:37:A:ILE:HD11	1:90:A:LYS:HD2	2	0.68	0.57	0.68
(1,1128)	1:37:A:ILE:HD12	1:90:A:LYS:HD2	2	0.68	0.57	0.68
(1,1128)	1:37:A:ILE:HD13	1:90:A:LYS:HD2	2	0.68	0.57	0.68
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB1	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB2	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB3	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB1	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB2	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB3	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB1	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB2	2	0.62	0.08	0.62
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB3	2	0.62	0.08	0.62
(1,1012)	1:151:A:GLN:HG3	1:113:A:ALA:H	2	0.6	0.28	0.6
(2,93)	1:88:A:TYR:HE1	1:103:A:VAL:HA	2	0.55	0.13	0.55
(2,93)	1:88:A:TYR:HE2	1:103:A:VAL:HA	2	0.55	0.13	0.55
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG11	2	0.53	0.39	0.53
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG12	2	0.53	0.39	0.53
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG13	2	0.53	0.39	0.53
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG11	2	0.53	0.39	0.53
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG12	2	0.53	0.39	0.53
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG13	2	0.53	0.39	0.53
(1,193)	1:151:A:GLN:H	1:151:A:GLN:HG3	2	0.52	0.0	0.52
(1,1815)	1:64:A:PRO:HB2	1:64:A:PRO:HD2	2	0.49	0.0	0.49
(1,1749)	1:104:A:LYS:HE2	1:157:A:ILE:HG21	2	0.48	0.15	0.48
(1,1631)	1:48:A:LEU:HD11	1:86:A:ARG:HB3	2	0.46	0.02	0.46
(1,1631)	1:48:A:LEU:HD12	1:86:A:ARG:HB3	2	0.46	0.02	0.46
(1,1631)	1:48:A:LEU:HD13	1:86:A:ARG:HB3	2	0.46	0.02	0.46
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG21	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG22	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG23	2	0.46	0.01	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG21	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG22	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG23	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG21	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG22	2	0.46	0.01	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG23	2	0.46	0.01	0.46
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG21	2	0.45	0.13	0.45
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG22	2	0.45	0.13	0.45
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG23	2	0.45	0.13	0.45
(1,1342)	1:92:A:LYS:HD2	1:92:A:LYS:H	2	0.44	0.07	0.44
(1,1458)	1:101:A:GLU:HG2	1:101:A:GLU:HA	2	0.41	0.02	0.41
(1,1411)	1:122:A:LYS:HG2	1:122:A:LYS:HA	2	0.4	0.1	0.4
(1,1072)	1:48:A:LEU:HD12	1:51:A:PHE:HD2	2	0.38	0.04	0.38
(1,1072)	1:48:A:LEU:HD13	1:51:A:PHE:HD2	2	0.38	0.04	0.38
(2,90)	1:88:A:TYR:HD1	1:159:A:HIS:HB3	2	0.37	0.2	0.37
(2,90)	1:88:A:TYR:HD2	1:159:A:HIS:HB3	2	0.37	0.2	0.37
(1,1079)	1:59:A:ALA:HB1	1:70:A:MET:H	2	0.36	0.01	0.36
(1,1079)	1:59:A:ALA:HB2	1:70:A:MET:H	2	0.36	0.01	0.36
(1,1079)	1:59:A:ALA:HB3	1:70:A:MET:H	2	0.36	0.01	0.36
(1,1497)	1:105:A:LEU:HD21	1:88:A:TYR:HA	2	0.35	0.11	0.35
(1,1497)	1:105:A:LEU:HD22	1:88:A:TYR:HA	2	0.35	0.11	0.35
(1,1497)	1:105:A:LEU:HD23	1:88:A:TYR:HA	2	0.35	0.11	0.35
(1,1758)	1:57:A:LYS:HE2	1:57:A:LYS:HG2	2	0.35	0.02	0.35
(1,1372)	1:177:A:VAL:HG21	1:118:A:ARG:HD3	2	0.34	0.0	0.34
(1,1372)	1:177:A:VAL:HG22	1:118:A:ARG:HD3	2	0.34	0.0	0.34
(1,1372)	1:177:A:VAL:HG23	1:118:A:ARG:HD3	2	0.34	0.0	0.34
(1,1471)	1:86:A:ARG:HD3	1:86:A:ARG:HA	2	0.34	0.1	0.34
(1,1471)	1:86:A:ARG:HD2	1:86:A:ARG:HA	2	0.34	0.1	0.34
(1,1334)	1:57:A:LYS:HE3	1:57:A:LYS:HG3	2	0.34	0.01	0.34
(1,1478)	1:176:A:GLN:HG2	1:176:A:GLN:HA	2	0.32	0.05	0.32
(1,147)	1:22:A:GLN:H	1:21:A:GLU:HA	2	0.32	0.16	0.32
(1,1495)	1:177:A:VAL:HG11	1:177:A:VAL:HA	2	0.29	0.0	0.29
(1,1495)	1:177:A:VAL:HG12	1:177:A:VAL:HA	2	0.29	0.0	0.29
(1,1495)	1:177:A:VAL:HG13	1:177:A:VAL:HA	2	0.29	0.0	0.29
(1,547)	1:97:A:PHE:H	1:92:A:LYS:HA	2	0.28	0.07	0.28
(1,598)	1:102:A:GLU:HB2	1:103:A:VAL:H	2	0.28	0.01	0.28
(1,1044)	1:99:A:PRO:HD3	1:99:A:PRO:HB2	2	0.28	0.01	0.28
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG11	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG12	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG13	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG11	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG12	2	0.27	0.05	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG13	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG11	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG12	2	0.27	0.05	0.27
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG13	2	0.27	0.05	0.27
(1,352)	1:57:A:LYS:H	1:57:A:LYS:HG2	2	0.26	0.02	0.26
(1,354)	1:58:A:ILE:H	1:57:A:LYS:HA	2	0.26	0.12	0.26
(1,2050)	1:177:A:VAL:HG11	2:2:B:C:H1'	2	0.25	0.01	0.25
(1,2050)	1:177:A:VAL:HG12	2:2:B:C:H1'	2	0.25	0.01	0.25
(1,2050)	1:177:A:VAL:HG13	2:2:B:C:H1'	2	0.25	0.01	0.25
(2,12)	1:71:A:VAL:H	1:73:A:ILE:H	2	0.24	0.08	0.24
(1,34)	1:57:A:LYS:H	1:72:A:VAL:H	2	0.24	0.02	0.24
(1,376)	1:57:A:LYS:H	1:57:A:LYS:HD2	2	0.24	0.09	0.24
(1,1924)	1:151:A:GLN:HG3	1:112:A:PRO:HA	2	0.24	0.03	0.24
(1,631)	1:176:A:GLN:HG3	1:176:A:GLN:H	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD11	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD12	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD13	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD11	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD12	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD13	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD11	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD12	2	0.22	0.01	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD13	2	0.22	0.01	0.22
(1,2051)	1:177:A:VAL:HG21	2:2:B:C:H1'	2	0.22	0.08	0.22
(1,2051)	1:177:A:VAL:HG22	2:2:B:C:H1'	2	0.22	0.08	0.22
(1,2051)	1:177:A:VAL:HG23	2:2:B:C:H1'	2	0.22	0.08	0.22
(2,45)	1:34:A:VAL:HG11	1:58:A:ILE:HA	2	0.22	0.02	0.22
(2,45)	1:34:A:VAL:HG12	1:58:A:ILE:HA	2	0.22	0.02	0.22
(2,45)	1:34:A:VAL:HG13	1:58:A:ILE:HA	2	0.22	0.02	0.22
(1,588)	1:58:A:ILE:HB	1:59:A:ALA:H	2	0.22	0.07	0.22
(1,481)	1:158:A:GLY:H	1:136:A:ALA:HA	2	0.22	0.02	0.22
(2,43)	1:157:A:ILE:HD11	1:105:A:LEU:HB2	2	0.22	0.02	0.22
(2,43)	1:157:A:ILE:HD12	1:105:A:LEU:HB2	2	0.22	0.02	0.22
(2,43)	1:157:A:ILE:HD13	1:105:A:LEU:HB2	2	0.22	0.02	0.22
(1,928)	1:47:A:GLN:HB2	1:47:A:GLN:HG3	2	0.2	0.0	0.2
(1,558)	1:83:A:ALA:H	1:86:A:ARG:HB2	2	0.2	0.09	0.2
(1,365)	1:102:A:GLU:H	1:102:A:GLU:HB3	2	0.2	0.09	0.2
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD11	2	0.19	0.07	0.19
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD12	2	0.19	0.07	0.19
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD13	2	0.19	0.07	0.19
(1,1732)	1:130:A:LEU:HD11	1:130:A:LEU:HB2	2	0.19	0.01	0.19
(1,1732)	1:130:A:LEU:HD12	1:130:A:LEU:HB2	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)
(1,1732)	1:130:A:LEU:HD13	1:130:A:LEU:HB2	2	0.19	0.01	0.19
(1,1538)	1:99:A:PRO:HA	1:99:A:PRO:HG3	2	0.18	0.0	0.18
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG11	2	0.16	0.06	0.16
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG12	2	0.16	0.06	0.16
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG13	2	0.16	0.06	0.16
(1,775)	1:150:A:GLU:HG3	1:150:A:GLU:HB2	2	0.16	0.03	0.16
(1,1125)	1:128:A:ASN:HB2	1:125:A:LYS:HA	2	0.16	0.03	0.16
(1,2077)	1:176:A:GLN:HA	1:179:A:GLN:H	2	0.16	0.02	0.16
(1,723)	1:111:A:VAL:HB	1:112:A:PRO:HD2	2	0.15	0.02	0.15
(1,1862)	1:63:A:THR:HB	1:64:A:PRO:HD2	2	0.15	0.01	0.15
(1,1940)	1:28:A:PHE:HD1	1:106:A:GLU:HB2	2	0.15	0.02	0.15
(1,1940)	1:28:A:PHE:HD2	1:106:A:GLU:HB2	2	0.15	0.02	0.15
(1,1945)	1:88:A:TYR:HD1	1:103:A:VAL:HB	2	0.15	0.01	0.15
(1,1945)	1:88:A:TYR:HD2	1:103:A:VAL:HB	2	0.15	0.01	0.15
(1,2061)	1:140:A:VAL:HA	1:154:A:VAL:HA	2	0.15	0.0	0.15
(1,301)	1:63:A:THR:H	1:62:A:GLU:HB2	2	0.15	0.0	0.15
(1,592)	1:58:A:ILE:HG21	1:58:A:ILE:H	2	0.15	0.04	0.15
(1,592)	1:58:A:ILE:HG22	1:58:A:ILE:H	2	0.15	0.04	0.15
(1,592)	1:58:A:ILE:HG23	1:58:A:ILE:H	2	0.15	0.04	0.15
(1,1167)	1:78:A:GLU:HG3	1:78:A:GLU:H	2	0.15	0.0	0.15
(1,940)	1:169:A:LYS:HA	1:172:A:ASP:HB2	2	0.14	0.01	0.14
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG21	2	0.14	0.02	0.14
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG22	2	0.14	0.02	0.14
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG23	2	0.14	0.02	0.14
(1,1908)	1:18:A:MET:HA	1:19:A:PRO:HD2	2	0.14	0.04	0.14
(1,1666)	1:145:A:THR:HG21	1:144:A:GLN:HA	2	0.13	0.0	0.13
(1,1666)	1:145:A:THR:HG22	1:144:A:GLN:HA	2	0.13	0.0	0.13
(1,1666)	1:145:A:THR:HG23	1:144:A:GLN:HA	2	0.13	0.0	0.13
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD11	2	0.12	0.01	0.12
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD12	2	0.12	0.01	0.12
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD13	2	0.12	0.01	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG21	2	0.12	0.0	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG22	2	0.12	0.0	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG23	2	0.12	0.0	0.12
(1,2097)	1:180:A:GLN:H	1:181:A:HIS:H	2	0.12	0.02	0.12
(1,453)	1:65:A:ASP:H	1:64:A:PRO:HB2	2	0.12	0.0	0.12
(1,274)	1:53:A:SER:H	1:53:A:SER:HB3	2	0.11	0.0	0.11
(1,1446)	1:145:A:THR:HG21	1:145:A:THR:HA	2	0.11	0.0	0.11
(1,1446)	1:145:A:THR:HG22	1:145:A:THR:HA	2	0.11	0.0	0.11
(1,1446)	1:145:A:THR:HG23	1:145:A:THR:HA	2	0.11	0.0	0.11
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD11	2	0.11	0.01	0.11
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD12	2	0.11	0.01	0.11

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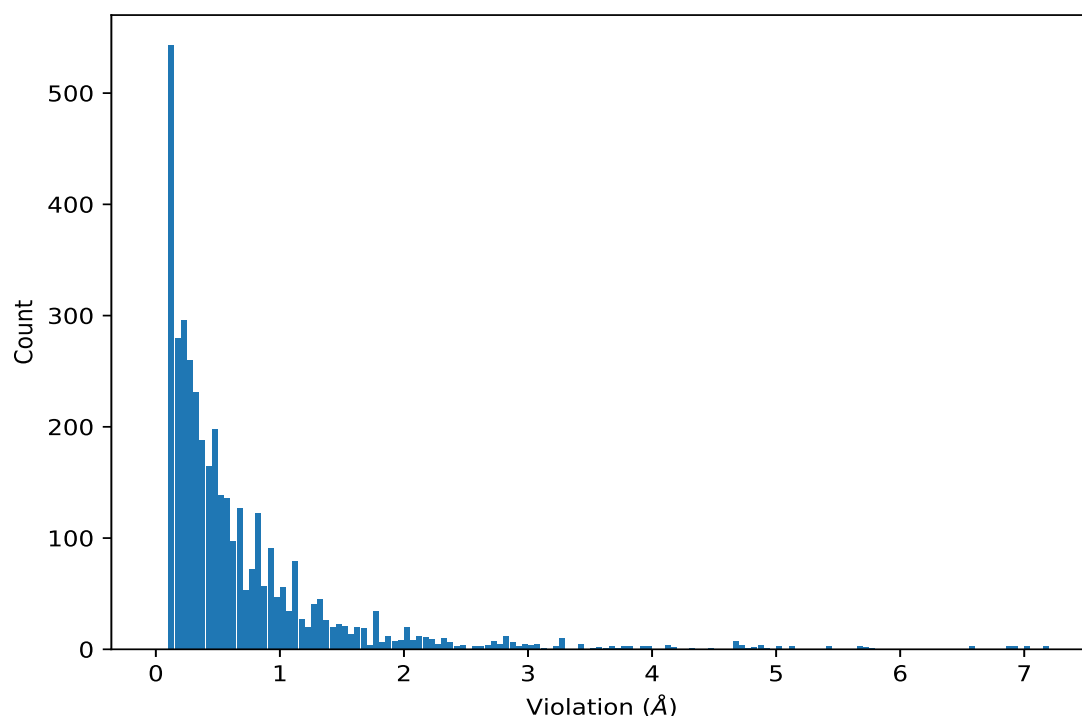
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD13	2	0.11	0.01	0.11
(1,2085)	1:168:A:ARG:H	1:169:A:LYS:H	2	0.11	0.0	0.11
(1,1800)	1:133:A:LEU:HD11	1:133:A:LEU:HB2	2	0.1	0.0	0.1
(1,1800)	1:133:A:LEU:HD12	1:133:A:LEU:HB2	2	0.1	0.0	0.1
(1,1800)	1:133:A:LEU:HD13	1:133:A:LEU:HB2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	5	7.18
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	5	7.18
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	5	7.18
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	11	7.02
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	11	7.02
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	11	7.02
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	10	6.9
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	10	6.9
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	10	6.9
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	9	6.89
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	9	6.89
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	9	6.89
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	8	6.56
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	8	6.56
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	8	6.56
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	4	5.8
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	6	5.73
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	5	5.72
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	7	5.69
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	9	5.67
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	9	5.67
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	4	5.41
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	4	5.41
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	4	5.41
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	8	5.13
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	10	5.12
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	10	5.12
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	4	5.04
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	4	5.04
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	4	5.04
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	1	4.93
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	2	4.87
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	2	4.87
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	2	4.87
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	10	4.87
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	11	4.84
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	11	4.84
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	7	4.77
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	9	4.71
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	9	4.71
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	9	4.71
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	3	4.7
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	9	4.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG2	10	4.65
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG2	10	4.65
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG2	10	4.65
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	5	4.65
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	5	4.65
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	5	4.65
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	5	4.46
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	6	4.32
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD1	9	4.15
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD2	9	4.15
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	3	4.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	7	4.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	7	4.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	7	4.14
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	6	3.95
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	6	3.95
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	6	3.95
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	1	3.91
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	1	3.91
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	1	3.91
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	6	3.82
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	6	3.82
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	6	3.82
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	3	3.77
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	3	3.77
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	3	3.77
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	1	3.72
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD1	10	3.69
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD2	10	3.69
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	3	3.66
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	11	3.62
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	2	3.58
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	10	3.57
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	11	3.51
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD1	11	3.43
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD2	11	3.43
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	6	3.42
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	6	3.42
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	6	3.42
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	3	3.3
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	3	3.3
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	3	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	11	3.29
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	11	3.29
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	11	3.29
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	6	3.28
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	6	3.28
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	6	3.28
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	2	3.26
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	2	3.24
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	2	3.24
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	2	3.24
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	4	3.11
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	8	3.09
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	8	3.09
(2,32)	1:63:A:THR:HG21	1:58:A:ILE:HA	1	3.06
(2,32)	1:63:A:THR:HG22	1:58:A:ILE:HA	1	3.06
(2,32)	1:63:A:THR:HG23	1:58:A:ILE:HA	1	3.06
(2,59)	1:102:A:GLU:HB2	1:136:A:ALA:HA	8	3.01
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	11	3.01
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	11	3.01
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	11	3.01
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	11	2.97
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	11	2.97
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	11	2.97
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	9	2.97
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	10	2.96
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG2	7	2.91
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG2	7	2.91
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG2	7	2.91
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	6	2.87
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	6	2.87
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	6	2.87
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	6	2.85
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	6	2.85
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	6	2.85
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	3	2.83
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	3	2.83
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	3	2.83
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	6	2.82
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	6	2.82
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	6	2.82
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	2	2.82
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	2	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	2	2.82
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD2	11	2.81
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD2	11	2.81
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD2	11	2.81
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	9	2.8
(1,1655)	1:31:A:ALA:HB1	1:67:A:LYS:HA	5	2.79
(1,1655)	1:31:A:ALA:HB2	1:67:A:LYS:HA	5	2.79
(1,1655)	1:31:A:ALA:HB3	1:67:A:LYS:HA	5	2.79
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	5	2.79
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	4	2.74
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG2	8	2.74
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG2	8	2.74
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	8	2.71
(1,1424)	1:103:A:VAL:HG21	1:159:A:HIS:HD2	10	2.7
(1,1424)	1:103:A:VAL:HG22	1:159:A:HIS:HD2	10	2.7
(1,1424)	1:103:A:VAL:HG23	1:159:A:HIS:HD2	10	2.7
(2,21)	1:63:A:THR:H	1:66:A:SER:HB2	5	2.68
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	3	2.68
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	3	2.68
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	3	2.68
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	2	2.65
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	2	2.65
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	2	2.65
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	10	2.59
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	10	2.59
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	10	2.59
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	10	2.48
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	10	2.45
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	10	2.45
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	10	2.45
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	8	2.42
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	8	2.42
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	8	2.42
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	11	2.39
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	6	2.38
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG2	12	2.37
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG2	12	2.37
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG2	12	2.37
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	8	2.36
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	10	2.34
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	10	2.34
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	10	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE1	6	2.33
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE2	6	2.33
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE1	6	2.33
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE2	6	2.33
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE1	6	2.33
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE2	6	2.33
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	3	2.31
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	11	2.3
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	11	2.3
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	11	2.3
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	9	2.28
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	10	2.26
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	5	2.23
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	5	2.23
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	5	2.23
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	6	2.21
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	6	2.21
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	6	2.21
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	1	2.21
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	1	2.21
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	1	2.21
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB1	7	2.19
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB2	7	2.19
(1,1817)	1:90:A:LYS:HE2	1:36:A:ALA:HB3	7	2.19
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG3	12	2.18
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	3	2.17
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	3	2.17
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	3	2.17
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	5	2.16
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	5	2.16
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	5	2.16
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	2	2.15
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG21	3	2.13
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG22	3	2.13
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG23	3	2.13
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG21	3	2.13
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG22	3	2.13
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG23	3	2.13
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG21	3	2.13
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG22	3	2.13
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG23	3	2.13
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	1	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	1	2.12
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	1	2.12
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	6	2.09
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	11	2.08
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	11	2.08
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	11	2.08
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	2	2.07
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	4	2.06
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	4	2.06
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	4	2.06
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	8	2.04
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	8	2.04
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	8	2.04
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG2	1	2.03
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	6	2.03
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	2	2.0
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	2	2.0
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	2	2.0
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD21	9	2.0
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD22	9	2.0
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD23	9	2.0
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD21	9	2.0
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD22	9	2.0
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD23	9	2.0
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD21	9	2.0
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD22	9	2.0
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD23	9	2.0
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	10	2.0
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	10	2.0
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	10	2.0
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	12	1.99
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	12	1.99
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	12	1.99
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	9	1.98
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	6	1.96
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	6	1.96
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	6	1.96
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG2	5	1.96
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	1	1.93
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	1	1.93
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	1	1.93
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	4	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	4	1.93
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	4	1.93
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	7	1.91
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	11	1.9
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	10	1.9
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	10	1.89
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	10	1.89
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	10	1.89
(1,642)	1:25:A:VAL:HG21	1:80:A:GLN:HE22	3	1.89
(1,642)	1:25:A:VAL:HG22	1:80:A:GLN:HE22	3	1.89
(1,642)	1:25:A:VAL:HG23	1:80:A:GLN:HE22	3	1.89
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	5	1.87
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	5	1.87
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	5	1.87
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	8	1.86
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	4	1.83
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	4	1.83
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	4	1.83
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	8	1.8
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	8	1.8
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	8	1.8
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	9	1.79
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	9	1.79
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	9	1.79
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD21	2	1.79
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD22	2	1.79
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD23	2	1.79
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD21	2	1.79
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD22	2	1.79
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD23	2	1.79
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD21	2	1.79
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD22	2	1.79
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD23	2	1.79
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	2	1.79
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	2	1.79
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	2	1.79
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	1	1.78
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	1	1.78
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	1	1.78
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	9	1.77
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	9	1.77
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	9	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD21	6	1.76
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD22	6	1.76
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD23	6	1.76
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD21	6	1.76
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD22	6	1.76
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD23	6	1.76
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	6	1.76
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	6	1.76
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	6	1.76
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	2	1.75
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	2	1.75
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	2	1.75
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	9	1.75
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG3	7	1.74
(1,2023)	1:118:A:ARG:HD3	2:2:B:C:H2'	6	1.72
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	4	1.71
(1,2065)	1:73:A:ILE:HA	1:56:A:ILE:HA	11	1.71
(1,1686)	1:113:A:ALA:HB2	1:150:A:GLU:HB3	10	1.7
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	4	1.7
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	4	1.7
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	1	1.69
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	1	1.69
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	1	1.69
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	5	1.69
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	5	1.69
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	5	1.69
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	5	1.68
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	5	1.68
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	5	1.68
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	11	1.68
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	11	1.68
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	11	1.68
(1,428)	1:150:A:GLU:H	1:151:A:GLN:HG3	3	1.68
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	3	1.66
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	3	1.66
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	3	1.66
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	3	1.64
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	3	1.64
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	3	1.64
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	11	1.64
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	5	1.63
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	11	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	11	1.63
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	11	1.63
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	9	1.63
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	9	1.63
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	9	1.63
(1,1742)	1:91:A:LEU:HD21	1:30:A:PRO:HD2	9	1.62
(1,1742)	1:91:A:LEU:HD22	1:30:A:PRO:HD2	9	1.62
(1,1742)	1:91:A:LEU:HD23	1:30:A:PRO:HD2	9	1.62
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	2	1.61
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	2	1.61
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	2	1.61
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	1	1.61
(2,7)	1:88:A:TYR:H	1:90:A:LYS:HD2	5	1.61
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	8	1.6
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	11	1.59
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	9	1.59
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	9	1.59
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	9	1.59
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	3	1.58
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	10	1.58
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	1	1.56
(1,1309)	1:91:A:LEU:HD21	1:96:A:PHE:HB2	6	1.56
(1,1309)	1:91:A:LEU:HD22	1:96:A:PHE:HB2	6	1.56
(1,1309)	1:91:A:LEU:HD23	1:96:A:PHE:HB2	6	1.56
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	1	1.56
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	1	1.56
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	1	1.56
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG3	2	1.55
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	1	1.53
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	1	1.53
(1,1782)	1:92:A:LYS:HE2	1:92:A:LYS:HB3	6	1.53
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	5	1.53
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG21	6	1.52
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG22	6	1.52
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG23	6	1.52
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	11	1.52
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	9	1.51
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	12	1.51
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	12	1.51
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	12	1.51
(1,506)	1:25:A:VAL:H	1:23:A:GLU:HG2	1	1.51
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	4	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	4	1.5
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	4	1.5
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	2	1.5
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	7	1.5
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	7	1.5
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	7	1.5
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	6	1.5
(1,1745)	1:28:A:PHE:HB2	1:106:A:GLU:HB2	1	1.49
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	5	1.48
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	5	1.48
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	5	1.48
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	4	1.48
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	4	1.48
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	4	1.48
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	2	1.48
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	2	1.48
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	2	1.48
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	10	1.48
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	10	1.48
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	10	1.48
(1,1684)	1:152:A:VAL:HG11	1:146:A:PRO:HA	12	1.47
(1,1684)	1:152:A:VAL:HG12	1:146:A:PRO:HA	12	1.47
(1,1684)	1:152:A:VAL:HG13	1:146:A:PRO:HA	12	1.47
(1,2065)	1:73:A:ILE:HA	1:56:A:ILE:HA	6	1.46
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	4	1.46
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	4	1.46
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	4	1.46
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	6	1.46
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	3	1.46
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	4	1.46
(1,1901)	1:153:A:ILE:HB	1:110:A:ARG:HD2	8	1.45
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	11	1.45
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	6	1.45
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	6	1.45
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	6	1.45
(2,81)	1:140:A:VAL:HG11	1:119:A:VAL:HA	7	1.44
(2,81)	1:140:A:VAL:HG12	1:119:A:VAL:HA	7	1.44
(2,81)	1:140:A:VAL:HG13	1:119:A:VAL:HA	7	1.44
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	7	1.44
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	7	1.44
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	7	1.44
(2,81)	1:140:A:VAL:HG11	1:119:A:VAL:HA	9	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:140:A:VAL:HG12	1:119:A:VAL:HA	9	1.43
(2,81)	1:140:A:VAL:HG13	1:119:A:VAL:HA	9	1.43
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	10	1.43
(1,2023)	1:118:A:ARG:HD3	2:2:B:C:H2'	7	1.42
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	7	1.42
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	2	1.42
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	2	1.42
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	2	1.42
(1,1656)	1:70:A:MET:HA	1:71:A:VAL:HG11	2	1.4
(1,1656)	1:70:A:MET:HA	1:71:A:VAL:HG12	2	1.4
(1,1656)	1:70:A:MET:HA	1:71:A:VAL:HG13	2	1.4
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD21	5	1.4
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD22	5	1.4
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD23	5	1.4
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD21	5	1.4
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD22	5	1.4
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD23	5	1.4
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD21	5	1.4
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD22	5	1.4
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD23	5	1.4
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	5	1.39
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	1	1.38
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	4	1.38
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	8	1.37
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	8	1.37
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	8	1.37
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	2	1.37
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	4	1.36
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	4	1.36
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	4	1.36
(1,1879)	1:92:A:LYS:HA	1:103:A:VAL:HG11	10	1.35
(1,1879)	1:92:A:LYS:HA	1:103:A:VAL:HG12	10	1.35
(1,1879)	1:92:A:LYS:HA	1:103:A:VAL:HG13	10	1.35
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	10	1.35
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	11	1.34
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	4	1.33
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	4	1.33
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	4	1.33
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	9	1.33
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	9	1.33
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	9	1.33
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	1	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	1	1.33
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	1	1.33
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	12	1.33
(1,1901)	1:153:A:ILE:HB	1:110:A:ARG:HD2	1	1.32
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	3	1.32
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	3	1.32
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	3	1.32
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	6	1.32
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	6	1.32
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	6	1.32
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	1	1.32
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	1	1.32
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	1	1.32
(2,101)	1:143:A:ASP:OD2	2:4:B:G:H21	6	1.31
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	10	1.31
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	10	1.31
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	10	1.31
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	9	1.31
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	9	1.31
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	9	1.31
(1,428)	1:150:A:GLU:H	1:151:A:GLN:HG3	2	1.31
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD11	7	1.3
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD12	7	1.3
(1,1889)	1:171:A:ARG:HD3	1:174:A:LEU:HD13	7	1.3
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	2	1.3
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	2	1.3
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	2	1.3
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	2	1.3
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	6	1.3
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	6	1.3
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	6	1.3
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	6	1.3
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	6	1.3
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	6	1.3
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	6	1.3
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	6	1.3
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	6	1.3
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	10	1.29
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	10	1.29
(1,1901)	1:153:A:ILE:HB	1:110:A:ARG:HD2	4	1.29
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	10	1.29
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	10	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	10	1.29
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	3	1.29
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	3	1.29
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	3	1.29
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	3	1.28
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	6	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	6	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	6	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	9	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	9	1.27
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	9	1.27
(2,69)	1:93:A:GLU:HB3	1:94:A:GLU:HB2	6	1.26
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	10	1.26
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	10	1.26
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	10	1.26
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	7	1.26
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	7	1.26
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	7	1.26
(1,1782)	1:92:A:LYS:HE3	1:92:A:LYS:HB3	12	1.26
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	7	1.26
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	8	1.26
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	8	1.26
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	8	1.26
(1,1128)	1:37:A:ILE:HD11	1:90:A:LYS:HD2	7	1.26
(1,1128)	1:37:A:ILE:HD12	1:90:A:LYS:HD2	7	1.26
(1,1128)	1:37:A:ILE:HD13	1:90:A:LYS:HD2	7	1.26
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	11	1.25
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	11	1.25
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	11	1.25
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	1	1.25
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	1	1.25
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	1	1.25
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	7	1.25
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	10	1.25
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	10	1.25
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	10	1.25
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	9	1.24
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	9	1.24
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	9	1.24
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	1	1.24
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	1	1.24
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	1	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG21	12	1.23
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG22	12	1.23
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG23	12	1.23
(1,1320)	1:131:A:GLN:HG3	1:135:A:ALA:HA	2	1.23
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	8	1.22
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	8	1.22
(1,1782)	1:92:A:LYS:HE2	1:92:A:LYS:HB3	3	1.22
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	10	1.22
(1,987)	1:63:A:THR:HG21	1:62:A:GLU:HB3	12	1.22
(1,987)	1:63:A:THR:HG22	1:62:A:GLU:HB3	12	1.22
(1,987)	1:63:A:THR:HG23	1:62:A:GLU:HB3	12	1.22
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD2	9	1.21
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD2	9	1.21
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD2	9	1.21
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	6	1.2
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	6	1.2
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	6	1.2
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	1	1.2
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	1	1.2
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	1	1.2
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	7	1.2
(1,111)	1:178:A:LYS:H	1:178:A:LYS:HG3	11	1.2
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	6	1.19
(2,64)	1:53:A:SER:HB2	1:82:A:LYS:HD2	4	1.19
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	7	1.19
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	8	1.19
(1,1951)	1:96:A:PHE:HD1	1:94:A:GLU:HB3	6	1.18
(1,1951)	1:96:A:PHE:HD2	1:94:A:GLU:HB3	6	1.18
(1,1730)	1:130:A:LEU:HB3	1:127:A:VAL:HA	6	1.18
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	10	1.18
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	12	1.17
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	12	1.17
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	12	1.17
(2,101)	1:143:A:ASP:OD2	2:4:B:G:H21	4	1.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD11	12	1.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD12	12	1.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD13	12	1.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD11	12	1.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD12	12	1.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD13	12	1.16
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	1	1.16
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	7	1.14
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	7	1.14
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG21	5	1.14
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG22	5	1.14
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG23	5	1.14
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	2	1.14
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	2	1.14
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	2	1.14
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	9	1.14
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	9	1.14
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	9	1.14
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	9	1.14
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	9	1.14
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	9	1.14
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	2	1.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB1	12	1.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB2	12	1.14
(1,1141)	1:102:A:GLU:HB3	1:135:A:ALA:HB3	12	1.14
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	4	1.13
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	5	1.13
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	5	1.13
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	5	1.13
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	8	1.13
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	3	1.13
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	5	1.13
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	5	1.13
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	5	1.13
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	5	1.13
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	5	1.13
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	5	1.13
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	5	1.13
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	5	1.13
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	5	1.13
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	5	1.12
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	5	1.12
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	5	1.12
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	1	1.12
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	1	1.12
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	1	1.12
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	3	1.12
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	3	1.12
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	10	1.12
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	10	1.12
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	10	1.12
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG2	5	1.12
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	8	1.12
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	4	1.12
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	4	1.12
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	4	1.12
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	4	1.12
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	4	1.12
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	4	1.12
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	8	1.12
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	8	1.12
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	8	1.12
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	6	1.11
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	6	1.11
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	6	1.11
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	10	1.11
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	10	1.11
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	10	1.11
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	10	1.1
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	10	1.1
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	10	1.1
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	10	1.1
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	10	1.1
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	10	1.1
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	10	1.1
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	10	1.1
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	10	1.1
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD3	11	1.1
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD3	11	1.1
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD3	11	1.1
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	3	1.1
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	3	1.1
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	3	1.1
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	3	1.1
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	1	1.09
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	9	1.09
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	9	1.09
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	9	1.09
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	9	1.09
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	9	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	9	1.09
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	9	1.09
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	9	1.09
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	9	1.09
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	6	1.09
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	6	1.09
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	6	1.09
(1,1686)	1:113:A:ALA:HB2	1:150:A:GLU:HB3	11	1.09
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	4	1.09
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD3	8	1.08
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD3	8	1.08
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD3	8	1.08
(1,1742)	1:91:A:LEU:HD21	1:30:A:PRO:HD2	3	1.08
(1,1742)	1:91:A:LEU:HD22	1:30:A:PRO:HD2	3	1.08
(1,1742)	1:91:A:LEU:HD23	1:30:A:PRO:HD2	3	1.08
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	10	1.07
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	2	1.07
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	2	1.07
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	2	1.07
(1,1686)	1:113:A:ALA:HB2	1:150:A:GLU:HB3	9	1.07
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	6	1.07
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	1	1.07
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	1	1.07
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	1	1.07
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	5	1.07
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	5	1.07
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	5	1.07
(1,1661)	1:105:A:LEU:HG	1:30:A:PRO:HD2	5	1.05
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	11	1.04
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	11	1.04
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	11	1.04
(1,428)	1:150:A:GLU:H	1:151:A:GLN:HG3	5	1.04
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	4	1.03
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	4	1.03
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	4	1.03
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	4	1.03
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	4	1.03
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	4	1.03
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	7	1.03
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	7	1.03
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	7	1.03
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	7	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:146:A:PRO:HD2	1:144:A:GLN:HG2	12	1.03
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	2	1.02
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	2	1.02
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	2	1.02
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	2	1.02
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	2	1.02
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	2	1.02
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	3	1.02
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	2	1.02
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	2	1.02
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	2	1.02
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	2	1.02
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	2	1.02
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	2	1.02
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	2	1.02
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	2	1.02
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	2	1.02
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	10	1.02
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	10	1.02
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	10	1.02
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	6	1.01
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	6	1.01
(1,1269)	1:58:A:ILE:HG12	1:58:A:ILE:H	11	1.01
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	5	1.01
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	5	1.01
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	5	1.01
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	2	1.0
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	5	1.0
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	5	1.0
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	11	1.0
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	11	1.0
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	11	1.0
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD1	11	1.0
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD2	11	1.0
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD1	11	1.0
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD2	11	1.0
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD1	11	1.0
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD2	11	1.0
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	5	1.0
(1,993)	1:154:A:VAL:HG11	1:153:A:ILE:HA	3	1.0
(1,993)	1:154:A:VAL:HG12	1:153:A:ILE:HA	3	1.0
(1,993)	1:154:A:VAL:HG13	1:153:A:ILE:HA	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	1	0.99
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	1	0.99
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	1	0.99
(1,993)	1:154:A:VAL:HG11	1:153:A:ILE:HA	2	0.99
(1,993)	1:154:A:VAL:HG12	1:153:A:ILE:HA	2	0.99
(1,993)	1:154:A:VAL:HG13	1:153:A:ILE:HA	2	0.99
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	12	0.98
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD1	9	0.98
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD2	9	0.98
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD1	12	0.98
(1,1365)	1:32:A:GLN:HG2	1:96:A:PHE:HD2	12	0.98
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	9	0.98
(1,145)	1:92:A:LYS:H	1:103:A:VAL:HG11	10	0.98
(1,145)	1:92:A:LYS:H	1:103:A:VAL:HG12	10	0.98
(1,145)	1:92:A:LYS:H	1:103:A:VAL:HG13	10	0.98
(2,81)	1:140:A:VAL:HG11	1:119:A:VAL:HA	5	0.97
(2,81)	1:140:A:VAL:HG12	1:119:A:VAL:HA	5	0.97
(2,81)	1:140:A:VAL:HG13	1:119:A:VAL:HA	5	0.97
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	12	0.97
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	3	0.97
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	3	0.97
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	3	0.97
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	3	0.97
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	3	0.97
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	6	0.97
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	6	0.97
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	6	0.97
(1,993)	1:154:A:VAL:HG11	1:153:A:ILE:HA	10	0.97
(1,993)	1:154:A:VAL:HG12	1:153:A:ILE:HA	10	0.97
(1,993)	1:154:A:VAL:HG13	1:153:A:ILE:HA	10	0.97
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	5	0.97
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	5	0.97
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	5	0.97
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	8	0.96
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	11	0.96
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	11	0.96
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD11	3	0.96
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD12	3	0.96
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD13	3	0.96
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD11	3	0.96
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD12	3	0.96
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD13	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD11	3	0.96
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD12	3	0.96
(1,1889)	1:171:A:ARG:HD2	1:174:A:LEU:HD13	3	0.96
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	7	0.96
(1,975)	1:57:A:LYS:HB2	1:72:A:VAL:HB	11	0.96
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	1	0.95
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD1	8	0.95
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD2	8	0.95
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD3	10	0.95
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD3	10	0.95
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD3	10	0.95
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	1	0.95
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	8	0.95
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	8	0.95
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	8	0.95
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	11	0.95
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	11	0.95
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	11	0.95
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	5	0.94
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	5	0.94
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	5	0.94
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD1	8	0.94
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD2	8	0.94
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD1	8	0.94
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD2	8	0.94
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD1	8	0.94
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD2	8	0.94
(1,1275)	1:92:A:LYS:HD2	1:92:A:LYS:HA	11	0.94
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	9	0.94
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	9	0.94
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	9	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	8	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	8	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	8	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	10	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	10	0.94
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	10	0.94
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	6	0.94
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	6	0.94
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	6	0.94
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	4	0.93
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	4	0.93
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	6	0.93
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	6	0.93
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	6	0.93
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG11	10	0.92
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG12	10	0.92
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG13	10	0.92
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG11	10	0.92
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG12	10	0.92
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG13	10	0.92
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG11	2	0.92
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG12	2	0.92
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG13	2	0.92
(1,1269)	1:58:A:ILE:HG12	1:58:A:ILE:H	10	0.92
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	5	0.92
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	5	0.92
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	5	0.92
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	2	0.92
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	2	0.92
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	2	0.92
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	11	0.91
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	7	0.91
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	7	0.91
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	7	0.91
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	9	0.91
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	9	0.91
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	9	0.91
(1,1309)	1:91:A:LEU:HD21	1:96:A:PHE:HB2	3	0.91
(1,1309)	1:91:A:LEU:HD22	1:96:A:PHE:HB2	3	0.91
(1,1309)	1:91:A:LEU:HD23	1:96:A:PHE:HB2	3	0.91
(1,1221)	1:146:A:PRO:HG3	1:144:A:GLN:HG3	5	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	1	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	1	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	1	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	9	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	9	0.91
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	9	0.91
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD1	10	0.9
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD2	10	0.9
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG21	4	0.9
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG22	4	0.9
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG23	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	6	0.9
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	6	0.9
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	6	0.9
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	2	0.9
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	2	0.9
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	2	0.9
(1,987)	1:63:A:THR:HG21	1:62:A:GLU:HB3	10	0.9
(1,987)	1:63:A:THR:HG22	1:62:A:GLU:HB3	10	0.9
(1,987)	1:63:A:THR:HG23	1:62:A:GLU:HB3	10	0.9
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	5	0.9
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	5	0.9
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	5	0.9
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	6	0.89
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	6	0.89
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	6	0.89
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	6	0.89
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	6	0.89
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	6	0.89
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG21	4	0.89
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG22	4	0.89
(1,1808)	1:54:A:ALA:HB1	1:73:A:ILE:HG23	4	0.89
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG21	4	0.89
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG22	4	0.89
(1,1808)	1:54:A:ALA:HB2	1:73:A:ILE:HG23	4	0.89
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG21	4	0.89
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG22	4	0.89
(1,1808)	1:54:A:ALA:HB3	1:73:A:ILE:HG23	4	0.89
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	2	0.89
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	2	0.89
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	2	0.89
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	11	0.89
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	11	0.89
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	11	0.89
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	11	0.89
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	11	0.89
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	11	0.89
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	11	0.89
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	11	0.89
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	11	0.89
(1,529)	1:111:A:VAL:H	1:152:A:VAL:HG21	12	0.89
(1,529)	1:111:A:VAL:H	1:152:A:VAL:HG22	12	0.89
(1,529)	1:111:A:VAL:H	1:152:A:VAL:HG23	12	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	11	0.88
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	11	0.88
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	11	0.88
(1,1622)	1:92:A:LYS:HE3	1:92:A:LYS:HG3	12	0.88
(1,1012)	1:151:A:GLN:HG3	1:113:A:ALA:H	3	0.88
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	2	0.87
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	2	0.87
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	10	0.87
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	10	0.87
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	10	0.87
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	7	0.87
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	7	0.87
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	7	0.87
(1,107)	1:178:A:LYS:H	1:177:A:VAL:HB	11	0.87
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	2	0.86
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	4	0.86
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	4	0.86
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	4	0.86
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	4	0.86
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	4	0.86
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	4	0.86
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	4	0.86
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	4	0.86
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	4	0.86
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	1	0.86
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	1	0.86
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	1	0.86
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	8	0.85
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	8	0.85
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	8	0.85
(1,1873)	1:178:A:LYS:HE2	1:178:A:LYS:HB3	2	0.85
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	3	0.85
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	3	0.85
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	3	0.85
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	11	0.85
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	11	0.85
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	11	0.85
(1,975)	1:57:A:LYS:HB2	1:72:A:VAL:HB	9	0.85
(2,64)	1:53:A:SER:HB2	1:82:A:LYS:HD2	8	0.84
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	1	0.84
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	1	0.84
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	1	0.84
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	1	0.84
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	1	0.84
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	1	0.84
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	1	0.84
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	1	0.84
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	7	0.84
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	7	0.84
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	7	0.84
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	6	0.84
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	6	0.84
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	6	0.84
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	4	0.84
(2,101)	1:143:A:ASP:OD2	2:4:B:G:H21	11	0.83
(1,1901)	1:153:A:ILE:HB	1:110:A:ARG:HD2	5	0.83
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD1	11	0.83
(1,1883)	1:33:A:ALA:HA	1:96:A:PHE:HD2	11	0.83
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	3	0.83
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	3	0.83
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	3	0.83
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE1	3	0.83
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE2	3	0.83
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE1	3	0.83
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE2	3	0.83
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE1	3	0.83
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE2	3	0.83
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	5	0.82
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	5	0.82
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	5	0.82
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	5	0.82
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	5	0.82
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	5	0.82
(1,1873)	1:178:A:LYS:HE2	1:178:A:LYS:HB3	5	0.82
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	8	0.82
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	8	0.82
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	8	0.82
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	10	0.82
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	10	0.82
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	10	0.82
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	8	0.82
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	8	0.82
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	1	0.82
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	1	0.82
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	1	0.82
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	4	0.81
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	4	0.81
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	4	0.81
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	3	0.81
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	3	0.81
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	3	0.81
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	3	0.81
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	3	0.81
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	3	0.81
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	3	0.81
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	3	0.81
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	3	0.81
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	5	0.81
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	5	0.81
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	5	0.81
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	7	0.81
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	7	0.81
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	7	0.81
(1,1118)	1:91:A:LEU:HD21	1:30:A:PRO:HD3	9	0.81
(1,1118)	1:91:A:LEU:HD22	1:30:A:PRO:HD3	9	0.81
(1,1118)	1:91:A:LEU:HD23	1:30:A:PRO:HD3	9	0.81
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	4	0.81
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	4	0.81
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	4	0.81
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	11	0.81
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	11	0.81
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	11	0.81
(1,437)	1:147:A:ASP:H	1:152:A:VAL:HG11	12	0.81
(1,437)	1:147:A:ASP:H	1:152:A:VAL:HG12	12	0.81
(1,437)	1:147:A:ASP:H	1:152:A:VAL:HG13	12	0.81
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	7	0.8
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	7	0.8
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	7	0.8
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	7	0.8
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	7	0.8
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD21	12	0.8
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD22	12	0.8
(1,1362)	1:27:A:VAL:HG21	1:105:A:LEU:HD23	12	0.8
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD21	12	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD22	12	0.8
(1,1362)	1:27:A:VAL:HG22	1:105:A:LEU:HD23	12	0.8
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD21	12	0.8
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD22	12	0.8
(1,1362)	1:27:A:VAL:HG23	1:105:A:LEU:HD23	12	0.8
(1,1318)	1:111:A:VAL:HG11	1:174:A:LEU:HD11	11	0.8
(1,1318)	1:111:A:VAL:HG11	1:174:A:LEU:HD12	11	0.8
(1,1318)	1:111:A:VAL:HG11	1:174:A:LEU:HD13	11	0.8
(1,1318)	1:111:A:VAL:HG12	1:174:A:LEU:HD11	11	0.8
(1,1318)	1:111:A:VAL:HG12	1:174:A:LEU:HD12	11	0.8
(1,1318)	1:111:A:VAL:HG12	1:174:A:LEU:HD13	11	0.8
(1,1318)	1:111:A:VAL:HG13	1:174:A:LEU:HD11	11	0.8
(1,1318)	1:111:A:VAL:HG13	1:174:A:LEU:HD12	11	0.8
(1,1318)	1:111:A:VAL:HG13	1:174:A:LEU:HD13	11	0.8
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG21	2	0.8
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG22	2	0.8
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG23	2	0.8
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG21	2	0.8
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG22	2	0.8
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG23	2	0.8
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG21	2	0.8
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG22	2	0.8
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG23	2	0.8
(2,88)	1:155:A:LYS:HE3	1:141:A:PRO:HB3	5	0.79
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	3	0.79
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	3	0.79
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	3	0.79
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	9	0.79
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	9	0.79
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	9	0.79
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	1	0.79
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	4	0.79
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	4	0.79
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	4	0.79
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	6	0.78
(1,1797)	1:110:A:ARG:HA	1:152:A:VAL:HG21	12	0.78
(1,1797)	1:110:A:ARG:HA	1:152:A:VAL:HG22	12	0.78
(1,1797)	1:110:A:ARG:HA	1:152:A:VAL:HG23	12	0.78
(1,1783)	1:116:A:ALA:HB1	1:140:A:VAL:HB	7	0.78
(1,1783)	1:116:A:ALA:HB2	1:140:A:VAL:HB	7	0.78
(1,1783)	1:116:A:ALA:HB3	1:140:A:VAL:HB	7	0.78
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:58:A:ILE:HG12	1:58:A:ILE:H	9	0.78
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	5	0.78
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	5	0.78
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	5	0.78
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	8	0.78
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	8	0.78
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	8	0.78
(1,987)	1:63:A:THR:HG21	1:62:A:GLU:HB3	1	0.78
(1,987)	1:63:A:THR:HG22	1:62:A:GLU:HB3	1	0.78
(1,987)	1:63:A:THR:HG23	1:62:A:GLU:HB3	1	0.78
(1,987)	1:63:A:THR:HG21	1:62:A:GLU:HB3	6	0.78
(1,987)	1:63:A:THR:HG22	1:62:A:GLU:HB3	6	0.78
(1,987)	1:63:A:THR:HG23	1:62:A:GLU:HB3	6	0.78
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG11	11	0.78
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG12	11	0.78
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG13	11	0.78
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	1	0.77
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	1	0.77
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	1	0.77
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	1	0.77
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	1	0.77
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	1	0.77
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	1	0.77
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	1	0.77
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	1	0.77
(1,107)	1:178:A:LYS:H	1:177:A:VAL:HB	8	0.77
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	12	0.76
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	12	0.76
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	12	0.76
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	3	0.76
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	3	0.76
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	3	0.76
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	6	0.76
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	6	0.76
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	6	0.76
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	7	0.76
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	9	0.75
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD1	8	0.75
(2,82)	1:32:A:GLN:HG3	1:96:A:PHE:HD2	8	0.75
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	6	0.75
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	3	0.75
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	3	0.75
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	5	0.75
(1,1119)	1:91:A:LEU:HD21	1:91:A:LEU:HA	6	0.75
(1,1119)	1:91:A:LEU:HD22	1:91:A:LEU:HA	6	0.75
(1,1119)	1:91:A:LEU:HD23	1:91:A:LEU:HA	6	0.75
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	6	0.75
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	6	0.75
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	6	0.75
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	7	0.75
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	7	0.75
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	7	0.75
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	6	0.74
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG21	4	0.74
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG22	4	0.74
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG23	4	0.74
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG21	4	0.74
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG22	4	0.74
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG23	4	0.74
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	2	0.74
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	2	0.74
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	2	0.74
(1,1632)	1:178:A:LYS:HE2	1:178:A:LYS:HG2	11	0.74
(1,1378)	1:142:A:ARG:HB2	1:141:A:PRO:HB3	3	0.74
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	3	0.74
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	3	0.74
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	3	0.74
(1,259)	1:94:A:GLU:H	1:94:A:GLU:HB2	6	0.74
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	10	0.73
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	10	0.73
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	10	0.73
(1,1320)	1:131:A:GLN:HG3	1:135:A:ALA:HA	7	0.73
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD1	10	0.73
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD2	10	0.73
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD1	10	0.73
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD2	10	0.73
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD1	10	0.73
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD2	10	0.73
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	2	0.73
(1,700)	1:128:A:ASN:HB3	1:125:A:LYS:HA	1	0.73
(1,700)	1:128:A:ASN:HB3	1:125:A:LYS:HA	6	0.73
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	5	0.72
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	5	0.72
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG21	5	0.72
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG22	5	0.72
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG23	5	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG21	5	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG22	5	0.72
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG23	5	0.72
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	4	0.72
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	4	0.72
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	4	0.72
(1,1320)	1:131:A:GLN:HG3	1:135:A:ALA:HA	8	0.72
(1,700)	1:128:A:ASN:HB3	1:125:A:LYS:HA	3	0.72
(1,1632)	1:178:A:LYS:HE3	1:178:A:LYS:HG2	10	0.71
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	9	0.71
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	9	0.71
(1,1269)	1:58:A:ILE:HG12	1:58:A:ILE:H	8	0.71
(1,1119)	1:91:A:LEU:HD21	1:91:A:LEU:HA	3	0.71
(1,1119)	1:91:A:LEU:HD22	1:91:A:LEU:HA	3	0.71
(1,1119)	1:91:A:LEU:HD23	1:91:A:LEU:HA	3	0.71
(1,454)	1:165:A:MET:H	1:164:A:GLN:HG2	7	0.71
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	6	0.71
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	2	0.71
(2,21)	1:63:A:THR:H	1:66:A:SER:HB2	2	0.7
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	3	0.7
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	3	0.7
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	3	0.7
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	3	0.7
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	3	0.7
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	3	0.7
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD3	4	0.7
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB1	1	0.7
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB2	1	0.7
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB3	1	0.7
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB1	1	0.7
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB2	1	0.7
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB3	1	0.7
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB1	1	0.7
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB2	1	0.7
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB3	1	0.7
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	2	0.7
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	2	0.7
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1378)	1:142:A:ARG:HB2	1:141:A:PRO:HB3	4	0.7
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	11	0.7
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	11	0.7
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	11	0.7
(1,1119)	1:91:A:LEU:HD21	1:91:A:LEU:HA	12	0.7
(1,1119)	1:91:A:LEU:HD22	1:91:A:LEU:HA	12	0.7
(1,1119)	1:91:A:LEU:HD23	1:91:A:LEU:HA	12	0.7
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	1	0.7
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	1	0.7
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	1	0.7
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	9	0.7
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	5	0.69
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	5	0.69
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	8	0.69
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	8	0.69
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	8	0.69
(1,762)	1:178:A:LYS:HA	1:181:A:HIS:HB3	12	0.69
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	7	0.69
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	7	0.69
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	7	0.69
(2,93)	1:88:A:TYR:HE1	1:103:A:VAL:HA	8	0.68
(2,93)	1:88:A:TYR:HE2	1:103:A:VAL:HA	8	0.68
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	11	0.68
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	11	0.68
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	11	0.68
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	4	0.68
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	4	0.68
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	4	0.68
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	7	0.68
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	7	0.68
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG21	3	0.68
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG22	3	0.68
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG23	3	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	9	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	9	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	9	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	10	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	10	0.68
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	10	0.68
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	6	0.67
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	6	0.67
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	6	0.67
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	6	0.67
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	6	0.67
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	6	0.67
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	6	0.67
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	6	0.67
(1,1563)	1:100:A:LYS:HA	1:100:A:LYS:HD3	8	0.67
(1,1014)	1:152:A:VAL:HG21	1:152:A:VAL:H	12	0.67
(1,1014)	1:152:A:VAL:HG22	1:152:A:VAL:H	12	0.67
(1,1014)	1:152:A:VAL:HG23	1:152:A:VAL:H	12	0.67
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	12	0.66
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	12	0.66
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	12	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	12	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	12	0.66
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	12	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	12	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	12	0.66
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	12	0.66
(1,1687)	1:113:A:ALA:HB1	1:152:A:VAL:HG11	12	0.66
(1,1687)	1:113:A:ALA:HB1	1:152:A:VAL:HG12	12	0.66
(1,1687)	1:113:A:ALA:HB1	1:152:A:VAL:HG13	12	0.66
(1,1687)	1:113:A:ALA:HB2	1:152:A:VAL:HG11	12	0.66
(1,1687)	1:113:A:ALA:HB2	1:152:A:VAL:HG12	12	0.66
(1,1687)	1:113:A:ALA:HB2	1:152:A:VAL:HG13	12	0.66
(1,1687)	1:113:A:ALA:HB3	1:152:A:VAL:HG11	12	0.66
(1,1687)	1:113:A:ALA:HB3	1:152:A:VAL:HG12	12	0.66
(1,1687)	1:113:A:ALA:HB3	1:152:A:VAL:HG13	12	0.66
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	4	0.66
(1,1419)	1:156:A:ILE:HG21	1:158:A:GLY:HA2	12	0.66
(1,1419)	1:156:A:ILE:HG22	1:158:A:GLY:HA2	12	0.66
(1,1419)	1:156:A:ILE:HG23	1:158:A:GLY:HA2	12	0.66
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG21	11	0.66
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG22	11	0.66
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG23	11	0.66
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG21	11	0.66
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG22	11	0.66
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG23	11	0.66
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG21	11	0.66
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG22	11	0.66
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG23	11	0.66
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	6	0.66
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	6	0.66
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	6	0.66
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	1	0.66
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	1	0.66
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	1	0.66
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	1	0.66
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	5	0.66
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	6	0.66
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	6	0.66
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	6	0.66
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG11	8	0.66
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG12	8	0.66
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG13	8	0.66
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	2	0.65
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	7	0.65
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	8	0.65
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	7	0.65
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	7	0.65
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	7	0.65
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	1	0.65
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	1	0.65
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	1	0.65
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG3	3	0.64
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG3	3	0.64
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	2	0.64
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	2	0.64
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	2	0.64
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	2	0.64
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	2	0.64
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	2	0.64
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	2	0.64
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	2	0.64
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	2	0.64
(1,1691)	1:110:A:ARG:HD2	1:151:A:GLN:HB2	1	0.64
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	1	0.64
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	5	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG21	9	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG22	9	0.64
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG23	9	0.64
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG21	9	0.64
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG22	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG23	9	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG21	9	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG22	9	0.64
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG23	9	0.64
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	12	0.64
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	12	0.64
(1,1216)	1:150:A:GLU:HG3	1:149:A:ASN:HA	9	0.64
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG21	3	0.64
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG22	3	0.64
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG23	3	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG21	3	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG22	3	0.64
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG23	3	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG21	3	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG22	3	0.64
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG23	3	0.64
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	4	0.64
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	1	0.64
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	1	0.63
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	1	0.63
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	1	0.63
(1,1749)	1:104:A:LYS:HE2	1:157:A:ILE:HG21	8	0.63
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	2	0.63
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	7	0.63
(1,1782)	1:92:A:LYS:HE2	1:92:A:LYS:HB3	7	0.62
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	5	0.62
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG21	10	0.62
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG22	10	0.62
(1,1391)	1:173:A:ILE:HD11	1:126:A:THR:HG23	10	0.62
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG21	10	0.62
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG22	10	0.62
(1,1391)	1:173:A:ILE:HD12	1:126:A:THR:HG23	10	0.62
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG21	10	0.62
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG22	10	0.62
(1,1391)	1:173:A:ILE:HD13	1:126:A:THR:HG23	10	0.62
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG21	1	0.62
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG22	1	0.62
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG23	1	0.62
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	3	0.62
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	6	0.62
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	6	0.62
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	9	0.62
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	9	0.62
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	9	0.62
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	9	0.62
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	9	0.62
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	9	0.62
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	9	0.62
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	9	0.62
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	9	0.62
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	1	0.62
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	1	0.62
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	1	0.62
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	3	0.62
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	3	0.62
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	3	0.62
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	4	0.62
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	4	0.62
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	4	0.62
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	5	0.62
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	5	0.62
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	5	0.62
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD2	9	0.62
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	3	0.62
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	2	0.61
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	9	0.61
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	9	0.61
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	11	0.61
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	11	0.61
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	11	0.61
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	2	0.61
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	2	0.61
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	2	0.61
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	3	0.61
(1,1490)	1:115:A:ALA:HB1	1:112:A:PRO:HD2	9	0.61
(1,1490)	1:115:A:ALA:HB2	1:112:A:PRO:HD2	9	0.61
(1,1490)	1:115:A:ALA:HB3	1:112:A:PRO:HD2	9	0.61
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	9	0.6
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	9	0.6
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	9	0.6
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG21	3	0.6
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG22	3	0.6
(1,1619)	1:106:A:GLU:HB2	1:157:A:ILE:HG23	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	7	0.6
(1,1119)	1:91:A:LEU:HD21	1:91:A:LEU:HA	9	0.6
(1,1119)	1:91:A:LEU:HD22	1:91:A:LEU:HA	9	0.6
(1,1119)	1:91:A:LEU:HD23	1:91:A:LEU:HA	9	0.6
(2,64)	1:53:A:SER:HB2	1:82:A:LYS:HD2	11	0.59
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD21	3	0.59
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD22	3	0.59
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD23	3	0.59
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD21	3	0.59
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD22	3	0.59
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD23	3	0.59
(1,1686)	1:113:A:ALA:HB1	1:150:A:GLU:HB3	6	0.59
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	6	0.59
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	6	0.59
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	4	0.59
(1,1220)	1:146:A:PRO:HD2	1:144:A:GLN:HG2	5	0.59
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	11	0.59
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	8	0.59
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	8	0.59
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	8	0.59
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	8	0.59
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	8	0.59
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	8	0.59
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	8	0.59
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	8	0.59
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	8	0.59
(1,1007)	1:157:A:ILE:HD11	1:106:A:GLU:HB3	10	0.59
(1,1007)	1:157:A:ILE:HD12	1:106:A:GLU:HB3	10	0.59
(1,1007)	1:157:A:ILE:HD13	1:106:A:GLU:HB3	10	0.59
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	5	0.58
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	5	0.58
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	5	0.58
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG2	7	0.58
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG11	3	0.58
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG12	3	0.58
(1,1615)	1:107:A:THR:HB	1:25:A:VAL:HG13	3	0.58
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	6	0.58
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	11	0.58
(1,1490)	1:115:A:ALA:HB1	1:112:A:PRO:HD2	10	0.58
(1,1490)	1:115:A:ALA:HB2	1:112:A:PRO:HD2	10	0.58
(1,1490)	1:115:A:ALA:HB3	1:112:A:PRO:HD2	10	0.58
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	2	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	2	0.58
(1,1357)	1:140:A:VAL:HG21	1:117:A:GLY:HA3	3	0.58
(1,1357)	1:140:A:VAL:HG22	1:117:A:GLY:HA3	3	0.58
(1,1357)	1:140:A:VAL:HG23	1:117:A:GLY:HA3	3	0.58
(1,1275)	1:92:A:LYS:HD2	1:92:A:LYS:HA	3	0.58
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG21	12	0.58
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG22	12	0.58
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG23	12	0.58
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	6	0.58
(1,975)	1:57:A:LYS:HB2	1:72:A:VAL:HB	6	0.58
(1,489)	1:172:A:ASP:H	1:171:A:ARG:HG3	11	0.58
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD3	3	0.58
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	12	0.58
(1,77)	1:102:A:GLU:H	1:101:A:GLU:HA	8	0.58
(2,90)	1:88:A:TYR:HD1	1:159:A:HIS:HB3	2	0.57
(2,90)	1:88:A:TYR:HD2	1:159:A:HIS:HB3	2	0.57
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG3	2	0.57
(1,1496)	1:87:A:ILE:HB	1:84:A:GLN:HA	1	0.57
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	8	0.57
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	8	0.57
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	8	0.57
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	6	0.57
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	6	0.57
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	6	0.57
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD2	6	0.57
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	10	0.57
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG21	11	0.56
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG22	11	0.56
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG23	11	0.56
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	8	0.56
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	8	0.56
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	8	0.56
(1,1634)	1:56:A:ILE:HG21	1:45:A:ILE:HG13	5	0.56
(1,1634)	1:56:A:ILE:HG22	1:45:A:ILE:HG13	5	0.56
(1,1634)	1:56:A:ILE:HG23	1:45:A:ILE:HG13	5	0.56
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	11	0.56
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	11	0.56
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	11	0.56
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	5	0.56
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	5	0.56
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	5	0.56
(1,1299)	1:102:A:GLU:HG3	1:102:A:GLU:H	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	7	0.56
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	7	0.56
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	7	0.56
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	9	0.56
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	9	0.56
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	9	0.56
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	2	0.56
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	2	0.56
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	2	0.56
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG11	12	0.56
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG12	12	0.56
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG13	12	0.56
(1,489)	1:172:A:ASP:H	1:171:A:ARG:HG3	10	0.56
(1,401)	1:170:A:ILE:H	1:170:A:ILE:HG12	2	0.56
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	2	0.55
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	2	0.55
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	2	0.55
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	12	0.55
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD2	9	0.55
(1,1622)	1:92:A:LYS:HE2	1:92:A:LYS:HG2	11	0.55
(1,1596)	1:116:A:ALA:HA	1:119:A:VAL:HG11	11	0.55
(1,1596)	1:116:A:ALA:HA	1:119:A:VAL:HG12	11	0.55
(1,1596)	1:116:A:ALA:HA	1:119:A:VAL:HG13	11	0.55
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB1	3	0.55
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB2	3	0.55
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB3	3	0.55
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB1	3	0.55
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB2	3	0.55
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB3	3	0.55
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB1	3	0.55
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB2	3	0.55
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB3	3	0.55
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	1	0.55
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	1	0.55
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	1	0.55
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	3	0.55
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	3	0.55
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	3	0.55
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	3	0.55
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	3	0.55
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	3	0.55
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	3	0.55
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	3	0.55
(1,489)	1:172:A:ASP:H	1:171:A:ARG:HG3	8	0.55
(1,454)	1:165:A:MET:H	1:164:A:GLN:HG2	6	0.55
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG21	3	0.54
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG22	3	0.54
(1,1959)	1:97:A:PHE:HD1	1:103:A:VAL:HG23	3	0.54
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG21	3	0.54
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG22	3	0.54
(1,1959)	1:97:A:PHE:HD2	1:103:A:VAL:HG23	3	0.54
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD2	3	0.54
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB1	12	0.54
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB2	12	0.54
(1,1864)	1:111:A:VAL:HG21	1:116:A:ALA:HB3	12	0.54
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB1	12	0.54
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB2	12	0.54
(1,1864)	1:111:A:VAL:HG22	1:116:A:ALA:HB3	12	0.54
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB1	12	0.54
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB2	12	0.54
(1,1864)	1:111:A:VAL:HG23	1:116:A:ALA:HB3	12	0.54
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	6	0.54
(1,1297)	1:100:A:LYS:HB2	1:100:A:LYS:H	8	0.54
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	2	0.53
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	4	0.53
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	9	0.53
(1,1501)	1:150:A:GLU:HG3	1:150:A:GLU:HA	10	0.53
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	8	0.53
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	8	0.53
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	8	0.53
(1,1299)	1:102:A:GLU:HG3	1:102:A:GLU:H	7	0.53
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG21	11	0.53
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG22	11	0.53
(1,1176)	1:154:A:VAL:HG11	1:111:A:VAL:HG23	11	0.53
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG21	11	0.53
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG22	11	0.53
(1,1176)	1:154:A:VAL:HG12	1:111:A:VAL:HG23	11	0.53
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG21	11	0.53
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG22	11	0.53
(1,1176)	1:154:A:VAL:HG13	1:111:A:VAL:HG23	11	0.53
(1,1118)	1:91:A:LEU:HD21	1:30:A:PRO:HD3	3	0.53
(1,1118)	1:91:A:LEU:HD22	1:30:A:PRO:HD3	3	0.53
(1,1118)	1:91:A:LEU:HD23	1:30:A:PRO:HD3	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:141:A:PRO:HD2	1:141:A:PRO:HB3	9	0.53
(1,762)	1:178:A:LYS:HA	1:181:A:HIS:HB3	5	0.53
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	3	0.52
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	3	0.52
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	3	0.52
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD2	5	0.52
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	7	0.52
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	7	0.52
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	7	0.52
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	7	0.52
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	7	0.52
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	7	0.52
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	7	0.52
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	7	0.52
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	7	0.52
(1,1791)	1:104:A:LYS:HE3	1:104:A:LYS:HB3	12	0.52
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	8	0.52
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	8	0.52
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	8	0.52
(1,1740)	1:91:A:LEU:HD21	1:94:A:GLU:HB3	7	0.52
(1,1740)	1:91:A:LEU:HD22	1:94:A:GLU:HB3	7	0.52
(1,1740)	1:91:A:LEU:HD23	1:94:A:GLU:HB3	7	0.52
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	3	0.52
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	3	0.52
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	3	0.52
(1,1022)	1:141:A:PRO:HD3	1:141:A:PRO:HB3	11	0.52
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	3	0.52
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	12	0.52
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	12	0.52
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	12	0.52
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	1	0.52
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	1	0.52
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	1	0.52
(1,193)	1:151:A:GLN:H	1:151:A:GLN:HG3	2	0.52
(1,193)	1:151:A:GLN:H	1:151:A:GLN:HG3	3	0.52
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	11	0.51
(1,1691)	1:110:A:ARG:HD2	1:151:A:GLN:HB2	3	0.51
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	9	0.51
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	9	0.51
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	9	0.51
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	7	0.51
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	7	0.51
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	5	0.51
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	5	0.51
(1,1342)	1:92:A:LYS:HD2	1:92:A:LYS:H	7	0.51
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	5	0.51
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	5	0.51
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	5	0.51
(1,988)	1:32:A:GLN:HG3	1:32:A:GLN:HB2	1	0.51
(1,988)	1:32:A:GLN:HG3	1:32:A:GLN:HB2	5	0.51
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	2	0.51
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	2	0.51
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	2	0.51
(1,587)	1:105:A:LEU:HD11	1:106:A:GLU:H	7	0.51
(1,587)	1:105:A:LEU:HD12	1:106:A:GLU:H	7	0.51
(1,587)	1:105:A:LEU:HD13	1:106:A:GLU:H	7	0.51
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	8	0.51
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	8	0.51
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	8	0.51
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD11	9	0.5
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD12	9	0.5
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD13	9	0.5
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD11	9	0.5
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD12	9	0.5
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD13	9	0.5
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD21	9	0.5
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD22	9	0.5
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD23	9	0.5
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD21	9	0.5
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD22	9	0.5
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD23	9	0.5
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	11	0.5
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	11	0.5
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	11	0.5
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	11	0.5
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	11	0.5
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	11	0.5
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	11	0.5
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	11	0.5
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	11	0.5
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	10	0.5
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	10	0.5
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:122:A:LYS:HG2	1:122:A:LYS:HA	8	0.5
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE1	9	0.5
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE2	9	0.5
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE1	9	0.5
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE2	9	0.5
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE1	9	0.5
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE2	9	0.5
(1,1022)	1:141:A:PRO:HD2	1:141:A:PRO:HB3	8	0.5
(1,700)	1:128:A:ASN:HB3	1:125:A:LYS:HA	12	0.5
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	10	0.5
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD3	4	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	2	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	2	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	2	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	5	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	5	0.5
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	5	0.5
(2,27)	1:56:A:ILE:HG21	1:45:A:ILE:HG12	6	0.49
(2,27)	1:56:A:ILE:HG22	1:45:A:ILE:HG12	6	0.49
(2,27)	1:56:A:ILE:HG23	1:45:A:ILE:HG12	6	0.49
(1,1815)	1:64:A:PRO:HB2	1:64:A:PRO:HD2	8	0.49
(1,1815)	1:64:A:PRO:HB2	1:64:A:PRO:HD2	11	0.49
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG11	1	0.49
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG12	1	0.49
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG13	1	0.49
(1,1663)	1:105:A:LEU:HD11	1:88:A:TYR:HA	6	0.49
(1,1663)	1:105:A:LEU:HD12	1:88:A:TYR:HA	6	0.49
(1,1663)	1:105:A:LEU:HD13	1:88:A:TYR:HA	6	0.49
(1,1479)	1:176:A:GLN:HG3	1:176:A:GLN:HA	3	0.49
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	6	0.49
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	6	0.49
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	6	0.49
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	11	0.49
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	11	0.49
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	8	0.49
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	8	0.49
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	8	0.49
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	11	0.49
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	11	0.49
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	11	0.49
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	1	0.49
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	2	0.49
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	2	0.49
(1,1022)	1:141:A:PRO:HD2	1:141:A:PRO:HB3	5	0.49
(1,489)	1:172:A:ASP:H	1:171:A:ARG:HG3	9	0.49
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	6	0.49
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	6	0.49
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	6	0.49
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	1	0.48
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	1	0.48
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	1	0.48
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG21	8	0.48
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG22	8	0.48
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG23	8	0.48
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	8	0.48
(1,1827)	1:176:A:GLN:HG3	1:175:A:ALA:HB1	3	0.48
(1,1827)	1:176:A:GLN:HG3	1:175:A:ALA:HB2	3	0.48
(1,1827)	1:176:A:GLN:HG3	1:175:A:ALA:HB3	3	0.48
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	8	0.48
(1,1631)	1:48:A:LEU:HD11	1:86:A:ARG:HB3	10	0.48
(1,1631)	1:48:A:LEU:HD12	1:86:A:ARG:HB3	10	0.48
(1,1631)	1:48:A:LEU:HD13	1:86:A:ARG:HB3	10	0.48
(1,1376)	1:151:A:GLN:HG3	1:149:A:ASN:HB2	9	0.48
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG21	5	0.48
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG22	5	0.48
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG23	5	0.48
(1,1022)	1:141:A:PRO:HD2	1:141:A:PRO:HB3	1	0.48
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	9	0.48
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	9	0.48
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	9	0.48
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG11	7	0.48
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG12	7	0.48
(1,502)	1:118:A:ARG:H	1:119:A:VAL:HG13	7	0.48
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	9	0.48
(1,424)	1:95:A:ASN:H	1:94:A:GLU:HG2	12	0.48
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	3	0.48
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	3	0.48
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	3	0.48
(1,1925)	1:151:A:GLN:HG2	1:112:A:PRO:HA	1	0.47
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG3	9	0.47
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	9	0.47
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	9	0.47
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	11	0.47
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	6	0.47
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	6	0.47
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	6	0.47
(1,1605)	1:45:A:ILE:HG21	1:58:A:ILE:HD11	11	0.47
(1,1605)	1:45:A:ILE:HG21	1:58:A:ILE:HD12	11	0.47
(1,1605)	1:45:A:ILE:HG21	1:58:A:ILE:HD13	11	0.47
(1,1605)	1:45:A:ILE:HG22	1:58:A:ILE:HD11	11	0.47
(1,1605)	1:45:A:ILE:HG22	1:58:A:ILE:HD12	11	0.47
(1,1605)	1:45:A:ILE:HG22	1:58:A:ILE:HD13	11	0.47
(1,1605)	1:45:A:ILE:HG23	1:58:A:ILE:HD11	11	0.47
(1,1605)	1:45:A:ILE:HG23	1:58:A:ILE:HD12	11	0.47
(1,1605)	1:45:A:ILE:HG23	1:58:A:ILE:HD13	11	0.47
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	7	0.47
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	7	0.47
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	7	0.47
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	7	0.47
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	7	0.47
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	7	0.47
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	7	0.47
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	7	0.47
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	7	0.47
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	2	0.47
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	2	0.47
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	2	0.47
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	5	0.47
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	5	0.47
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	5	0.47
(1,1299)	1:102:A:GLU:HG2	1:102:A:GLU:H	4	0.47
(1,1299)	1:102:A:GLU:HG2	1:102:A:GLU:H	5	0.47
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	6	0.47
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	10	0.47
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	10	0.47
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	10	0.47
(1,988)	1:32:A:GLN:HG3	1:32:A:GLN:HB2	9	0.47
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	2	0.47
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	8	0.47
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	1	0.47
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	1	0.47
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	1	0.47
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG11	4	0.47
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG12	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:34:A:VAL:H	1:34:A:VAL:HG13	4	0.47
(1,147)	1:22:A:GLN:H	1:21:A:GLU:HA	4	0.47
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG21	1	0.46
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG22	1	0.46
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG23	1	0.46
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG21	1	0.46
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG22	1	0.46
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG23	1	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG21	1	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG22	1	0.46
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG23	1	0.46
(1,1497)	1:105:A:LEU:HD21	1:88:A:TYR:HA	9	0.46
(1,1497)	1:105:A:LEU:HD22	1:88:A:TYR:HA	9	0.46
(1,1497)	1:105:A:LEU:HD23	1:88:A:TYR:HA	9	0.46
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	1	0.46
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	1	0.46
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	1	0.46
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	4	0.46
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	4	0.46
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	4	0.46
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	6	0.46
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	10	0.46
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	10	0.46
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	10	0.46
(1,1353)	1:37:A:ILE:HG21	1:87:A:ILE:HG12	10	0.46
(1,1353)	1:37:A:ILE:HG22	1:87:A:ILE:HG12	10	0.46
(1,1353)	1:37:A:ILE:HG23	1:87:A:ILE:HG12	10	0.46
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD2	2	0.46
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD2	2	0.46
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD2	2	0.46
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	5	0.46
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	5	0.46
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	5	0.46
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	12	0.46
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	12	0.46
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	12	0.46
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	10	0.46
(1,520)	1:149:A:ASN:HD22	1:149:A:ASN:H	9	0.46
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG11	12	0.46
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG12	12	0.46
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG13	12	0.46
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD3	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD2	11	0.46
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	9	0.46
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	4	0.45
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	4	0.45
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG21	9	0.45
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG22	9	0.45
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG23	9	0.45
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	8	0.45
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	8	0.45
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	8	0.45
(1,1783)	1:116:A:ALA:HB1	1:140:A:VAL:HB	6	0.45
(1,1783)	1:116:A:ALA:HB2	1:140:A:VAL:HB	6	0.45
(1,1783)	1:116:A:ALA:HB3	1:140:A:VAL:HB	6	0.45
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	7	0.45
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	7	0.45
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	7	0.45
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	2	0.45
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG21	12	0.45
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG22	12	0.45
(1,1606)	1:115:A:ALA:HB1	1:111:A:VAL:HG23	12	0.45
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG21	12	0.45
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG22	12	0.45
(1,1606)	1:115:A:ALA:HB2	1:111:A:VAL:HG23	12	0.45
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG21	12	0.45
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG22	12	0.45
(1,1606)	1:115:A:ALA:HB3	1:111:A:VAL:HG23	12	0.45
(1,1490)	1:115:A:ALA:HB1	1:112:A:PRO:HD2	8	0.45
(1,1490)	1:115:A:ALA:HB2	1:112:A:PRO:HD2	8	0.45
(1,1490)	1:115:A:ALA:HB3	1:112:A:PRO:HD2	8	0.45
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	5	0.45
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	8	0.45
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	11	0.45
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	3	0.45
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	3	0.45
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	11	0.45
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	11	0.45
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	11	0.45
(1,830)	1:171:A:ARG:HA	1:174:A:LEU:HB3	9	0.45
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	6	0.45
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	6	0.45
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	6	0.45
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	5	0.45
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG11	11	0.45
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG12	11	0.45
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG13	11	0.45
(1,389)	1:100:A:LYS:H	1:100:A:LYS:HD2	5	0.45
(2,81)	1:140:A:VAL:HG11	1:119:A:VAL:HA	6	0.44
(2,81)	1:140:A:VAL:HG12	1:119:A:VAL:HA	6	0.44
(2,81)	1:140:A:VAL:HG13	1:119:A:VAL:HA	6	0.44
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD11	12	0.44
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD12	12	0.44
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD13	12	0.44
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD11	12	0.44
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD12	12	0.44
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD13	12	0.44
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	8	0.44
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	8	0.44
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	8	0.44
(1,1631)	1:48:A:LEU:HD11	1:86:A:ARG:HB3	4	0.44
(1,1631)	1:48:A:LEU:HD12	1:86:A:ARG:HB3	4	0.44
(1,1631)	1:48:A:LEU:HD13	1:86:A:ARG:HB3	4	0.44
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	1	0.44
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	1	0.44
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	1	0.44
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	1	0.44
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	1	0.44
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	1	0.44
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	1	0.44
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	1	0.44
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	1	0.44
(1,1490)	1:115:A:ALA:HB1	1:112:A:PRO:HD2	11	0.44
(1,1490)	1:115:A:ALA:HB2	1:112:A:PRO:HD2	11	0.44
(1,1490)	1:115:A:ALA:HB3	1:112:A:PRO:HD2	11	0.44
(1,1471)	1:86:A:ARG:HD2	1:86:A:ARG:HA	4	0.44
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	1	0.44
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	9	0.44
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	9	0.44
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	9	0.44
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	9	0.44
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	3	0.44
(1,634)	1:34:A:VAL:HG11	1:33:A:ALA:H	2	0.44
(1,634)	1:34:A:VAL:HG12	1:33:A:ALA:H	2	0.44
(1,634)	1:34:A:VAL:HG13	1:33:A:ALA:H	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:179:A:GLN:H	1:176:A:GLN:HA	8	0.44
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB3	10	0.43
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG11	6	0.43
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG12	6	0.43
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG13	6	0.43
(1,1458)	1:101:A:GLU:HG2	1:101:A:GLU:HA	8	0.43
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	1	0.43
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	1	0.43
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	1	0.43
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	2	0.43
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	3	0.43
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	10	0.43
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	4	0.43
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	4	0.43
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	4	0.43
(1,852)	1:100:A:LYS:HA	1:100:A:LYS:HG2	8	0.43
(1,762)	1:178:A:LYS:HA	1:181:A:HIS:HB3	9	0.43
(1,589)	1:57:A:LYS:HB2	1:57:A:LYS:H	9	0.43
(1,483)	1:143:A:ASP:H	1:142:A:ARG:HG2	3	0.43
(1,483)	1:143:A:ASP:H	1:142:A:ARG:HG2	12	0.43
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG11	8	0.43
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG12	8	0.43
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG13	8	0.43
(2,93)	1:88:A:TYR:HE1	1:103:A:VAL:HA	11	0.42
(2,93)	1:88:A:TYR:HE2	1:103:A:VAL:HA	11	0.42
(1,1939)	1:28:A:PHE:HD1	1:106:A:GLU:HG2	10	0.42
(1,1939)	1:28:A:PHE:HD2	1:106:A:GLU:HG2	10	0.42
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	3	0.42
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	3	0.42
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	3	0.42
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	3	0.42
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	3	0.42
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	3	0.42
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	3	0.42
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	3	0.42
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	3	0.42
(1,1742)	1:91:A:LEU:HD21	1:30:A:PRO:HD2	6	0.42
(1,1742)	1:91:A:LEU:HD22	1:30:A:PRO:HD2	6	0.42
(1,1742)	1:91:A:LEU:HD23	1:30:A:PRO:HD2	6	0.42
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	12	0.42
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	12	0.42
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	6	0.42
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	6	0.42
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	6	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	6	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	6	0.42
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	6	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	6	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	6	0.42
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	6	0.42
(1,1469)	1:32:A:GLN:HG3	1:32:A:GLN:HA	11	0.42
(1,1299)	1:102:A:GLU:HG2	1:102:A:GLU:H	6	0.42
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	5	0.42
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	5	0.42
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	5	0.42
(1,1072)	1:48:A:LEU:HD13	1:51:A:PHE:HD2	12	0.42
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	1	0.42
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	11	0.41
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG3	5	0.41
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG3	5	0.41
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	9	0.41
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	9	0.41
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	9	0.41
(1,1717)	1:50:A:ARG:HD2	1:50:A:ARG:HB3	5	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	1	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	1	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	1	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	1	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	1	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	1	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	1	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	1	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	1	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	2	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	2	0.41
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	2	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	2	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	2	0.41
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	2	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	2	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	2	0.41
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	2	0.41
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	8	0.41
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	8	0.41
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	8	0.41
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	8	0.41
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	8	0.41
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	8	0.41
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	8	0.41
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	8	0.41
(1,1404)	1:61:A:PRO:HB2	1:61:A:PRO:HD2	4	0.41
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG2	12	0.41
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG21	11	0.41
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG22	11	0.41
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG23	11	0.41
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG21	11	0.41
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG22	11	0.41
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG23	11	0.41
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG21	11	0.41
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG22	11	0.41
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG23	11	0.41
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	3	0.41
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG11	7	0.41
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG12	7	0.41
(1,467)	1:119:A:VAL:H	1:119:A:VAL:HG13	7	0.41
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	11	0.41
(1,1948)	1:96:A:PHE:HD1	1:91:A:LEU:HA	6	0.4
(1,1948)	1:96:A:PHE:HD2	1:91:A:LEU:HA	6	0.4
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	12	0.4
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	10	0.4
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	10	0.4
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	10	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	10	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	10	0.4
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	10	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	10	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	10	0.4
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	10	0.4
(1,1299)	1:102:A:GLU:HG2	1:102:A:GLU:H	2	0.4
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	12	0.4
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	12	0.4
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	12	0.4
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	8	0.4
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	8	0.4
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	5	0.4
(2,50)	1:152:A:VAL:HG21	1:117:A:GLY:H	12	0.39
(2,50)	1:152:A:VAL:HG22	1:117:A:GLY:H	12	0.39
(2,50)	1:152:A:VAL:HG23	1:117:A:GLY:H	12	0.39
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	3	0.39
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	3	0.39
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	3	0.39
(1,1782)	1:92:A:LYS:HE3	1:92:A:LYS:HB3	5	0.39
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG21	6	0.39
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG22	6	0.39
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG23	6	0.39
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	10	0.39
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	10	0.39
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	10	0.39
(1,1746)	1:37:A:ILE:HD11	1:87:A:ILE:HA	7	0.39
(1,1746)	1:37:A:ILE:HD12	1:87:A:ILE:HA	7	0.39
(1,1746)	1:37:A:ILE:HD13	1:87:A:ILE:HA	7	0.39
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	1	0.39
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	1	0.39
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	1	0.39
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	2	0.39
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	2	0.39
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	2	0.39
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	3	0.39
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	3	0.39
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	3	0.39
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	5	0.39
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	5	0.39
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	5	0.39
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	9	0.39
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	9	0.39
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	9	0.39
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	9	0.39
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	9	0.39
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	9	0.39
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	9	0.39
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	9	0.39
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	9	0.39
(1,1469)	1:32:A:GLN:HG3	1:32:A:GLN:HA	10	0.39
(1,1458)	1:101:A:GLU:HG2	1:101:A:GLU:HA	9	0.39
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	5	0.39
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	5	0.39
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	4	0.39
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	4	0.39
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	4	0.39
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	10	0.39
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	10	0.39
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	10	0.39
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	11	0.38
(1,1939)	1:28:A:PHE:HD1	1:106:A:GLU:HG2	1	0.38
(1,1939)	1:28:A:PHE:HD2	1:106:A:GLU:HG2	1	0.38
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB3	7	0.38
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	2	0.38
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	2	0.38
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	2	0.38
(1,1793)	1:109:A:ILE:HG21	1:107:A:THR:HG21	4	0.38
(1,1793)	1:109:A:ILE:HG21	1:107:A:THR:HG22	4	0.38
(1,1793)	1:109:A:ILE:HG21	1:107:A:THR:HG23	4	0.38
(1,1793)	1:109:A:ILE:HG22	1:107:A:THR:HG21	4	0.38
(1,1793)	1:109:A:ILE:HG22	1:107:A:THR:HG22	4	0.38
(1,1793)	1:109:A:ILE:HG22	1:107:A:THR:HG23	4	0.38
(1,1793)	1:109:A:ILE:HG23	1:107:A:THR:HG21	4	0.38
(1,1793)	1:109:A:ILE:HG23	1:107:A:THR:HG22	4	0.38
(1,1793)	1:109:A:ILE:HG23	1:107:A:THR:HG23	4	0.38
(1,1756)	1:57:A:LYS:HE3	1:57:A:LYS:HB2	5	0.38
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	11	0.38
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	11	0.38
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	11	0.38
(1,1720)	1:50:A:ARG:HD3	1:50:A:ARG:HA	9	0.38
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	9	0.38
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	9	0.38
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	9	0.38
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	11	0.38
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	11	0.38
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	11	0.38
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	11	0.38
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	11	0.38
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	11	0.38
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	11	0.38
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	11	0.38
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	11	0.38
(1,1478)	1:176:A:GLN:HG2	1:176:A:GLN:HA	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	3	0.38
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	3	0.38
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	3	0.38
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	3	0.38
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	3	0.38
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	3	0.38
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD11	2	0.38
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD12	2	0.38
(1,1074)	1:48:A:LEU:HD11	1:56:A:ILE:HD13	2	0.38
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD11	2	0.38
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD12	2	0.38
(1,1074)	1:48:A:LEU:HD12	1:56:A:ILE:HD13	2	0.38
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD11	2	0.38
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD12	2	0.38
(1,1074)	1:48:A:LEU:HD13	1:56:A:ILE:HD13	2	0.38
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	2	0.38
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	2	0.38
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	2	0.38
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	11	0.38
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	9	0.37
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD11	10	0.37
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD12	10	0.37
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD13	10	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD11	10	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD12	10	0.37
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD13	10	0.37
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB1	12	0.37
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB2	12	0.37
(1,1817)	1:90:A:LYS:HE3	1:36:A:ALA:HB3	12	0.37
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	2	0.37
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	5	0.37
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	5	0.37
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	5	0.37
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG21	2	0.37
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG22	2	0.37
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG23	2	0.37
(1,1758)	1:57:A:LYS:HE2	1:57:A:LYS:HG2	1	0.37
(1,1727)	1:58:A:ILE:HG21	1:58:A:ILE:HG12	11	0.37
(1,1727)	1:58:A:ILE:HG22	1:58:A:ILE:HG12	11	0.37
(1,1727)	1:58:A:ILE:HG23	1:58:A:ILE:HG12	11	0.37
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	6	0.37
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	6	0.37
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	8	0.37
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	8	0.37
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	8	0.37
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB1	5	0.37
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB2	5	0.37
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB3	5	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB1	5	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB2	5	0.37
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB3	5	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB1	5	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB2	5	0.37
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB3	5	0.37
(1,1412)	1:171:A:ARG:HB3	1:168:A:ARG:HA	5	0.37
(1,1342)	1:92:A:LYS:HD2	1:92:A:LYS:H	11	0.37
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	2	0.37
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	2	0.37
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	2	0.37
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	2	0.37
(1,1079)	1:59:A:ALA:HB1	1:70:A:MET:H	11	0.37
(1,1079)	1:59:A:ALA:HB2	1:70:A:MET:H	11	0.37
(1,1079)	1:59:A:ALA:HB3	1:70:A:MET:H	11	0.37
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	1	0.37
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	1	0.37
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	1	0.37
(1,354)	1:58:A:ILE:H	1:57:A:LYS:HA	6	0.37
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	6	0.36
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	6	0.36
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	6	0.36
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	7	0.36
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	7	0.36
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	7	0.36
(1,1776)	1:56:A:ILE:HD11	1:71:A:VAL:HB	5	0.36
(1,1776)	1:56:A:ILE:HD12	1:71:A:VAL:HB	5	0.36
(1,1776)	1:56:A:ILE:HD13	1:71:A:VAL:HB	5	0.36
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	4	0.36
(1,1722)	1:76:A:PRO:HB2	1:77:A:PRO:HG2	9	0.36
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	4	0.36
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	4	0.36
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	4	0.36
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	4	0.36
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	4	0.36
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	4	0.36
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	4	0.36
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	4	0.36
(1,1469)	1:32:A:GLN:HG3	1:32:A:GLN:HA	12	0.36
(1,1319)	1:130:A:LEU:HD11	1:166:A:ALA:HB1	9	0.36
(1,1319)	1:130:A:LEU:HD11	1:166:A:ALA:HB2	9	0.36
(1,1319)	1:130:A:LEU:HD11	1:166:A:ALA:HB3	9	0.36
(1,1319)	1:130:A:LEU:HD12	1:166:A:ALA:HB1	9	0.36
(1,1319)	1:130:A:LEU:HD12	1:166:A:ALA:HB2	9	0.36
(1,1319)	1:130:A:LEU:HD12	1:166:A:ALA:HB3	9	0.36
(1,1319)	1:130:A:LEU:HD13	1:166:A:ALA:HB1	9	0.36
(1,1319)	1:130:A:LEU:HD13	1:166:A:ALA:HB2	9	0.36
(1,1319)	1:130:A:LEU:HD13	1:166:A:ALA:HB3	9	0.36
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	4	0.36
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	4	0.36
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	4	0.36
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	9	0.36
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	9	0.36
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	9	0.36
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	4	0.36
(1,454)	1:165:A:MET:H	1:164:A:GLN:HG2	1	0.36
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	1	0.35
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	1	0.35
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	1	0.35
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	1	0.35
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	1	0.35
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	1	0.35
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG3	11	0.35
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG3	11	0.35
(1,1944)	1:88:A:TYR:HD1	1:84:A:GLN:HB2	3	0.35
(1,1944)	1:88:A:TYR:HD2	1:84:A:GLN:HB2	3	0.35
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB3	9	0.35
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	3	0.35
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	3	0.35
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	3	0.35
(1,1707)	1:48:A:LEU:HD11	1:48:A:LEU:HB3	11	0.35
(1,1707)	1:48:A:LEU:HD12	1:48:A:LEU:HB3	11	0.35
(1,1707)	1:48:A:LEU:HD13	1:48:A:LEU:HB3	11	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	6	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	6	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	6	0.35
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	6	0.35
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	6	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	6	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	6	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	6	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD11	8	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD12	8	0.35
(1,1701)	1:54:A:ALA:HB1	1:73:A:ILE:HD13	8	0.35
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD11	8	0.35
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD12	8	0.35
(1,1701)	1:54:A:ALA:HB2	1:73:A:ILE:HD13	8	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD11	8	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD12	8	0.35
(1,1701)	1:54:A:ALA:HB3	1:73:A:ILE:HD13	8	0.35
(1,1691)	1:110:A:ARG:HD2	1:151:A:GLN:HB2	2	0.35
(1,1691)	1:110:A:ARG:HD2	1:151:A:GLN:HB2	6	0.35
(1,1663)	1:105:A:LEU:HD11	1:88:A:TYR:HA	3	0.35
(1,1663)	1:105:A:LEU:HD12	1:88:A:TYR:HA	3	0.35
(1,1663)	1:105:A:LEU:HD13	1:88:A:TYR:HA	3	0.35
(1,1380)	1:141:A:PRO:HG2	1:144:A:GLN:HA	1	0.35
(1,1372)	1:177:A:VAL:HG21	1:118:A:ARG:HD3	11	0.35
(1,1372)	1:177:A:VAL:HG22	1:118:A:ARG:HD3	11	0.35
(1,1372)	1:177:A:VAL:HG23	1:118:A:ARG:HD3	11	0.35
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	3	0.35
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD3	11	0.35
(1,1275)	1:92:A:LYS:HD2	1:92:A:LYS:HA	8	0.35
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	3	0.35
(1,1072)	1:48:A:LEU:HD12	1:51:A:PHE:HD2	4	0.35
(1,539)	1:179:A:GLN:H	1:176:A:GLN:HA	11	0.35
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	2	0.35
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG3	10	0.34
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG3	10	0.34
(1,1957)	1:97:A:PHE:HD1	1:91:A:LEU:HB3	1	0.34
(1,1957)	1:97:A:PHE:HD2	1:91:A:LEU:HB3	1	0.34
(1,1939)	1:28:A:PHE:HD1	1:106:A:GLU:HG2	2	0.34
(1,1939)	1:28:A:PHE:HD2	1:106:A:GLU:HG2	2	0.34
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG21	5	0.34
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG22	5	0.34
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG23	5	0.34
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	2	0.34
(1,1783)	1:116:A:ALA:HB1	1:140:A:VAL:HB	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:116:A:ALA:HB2	1:140:A:VAL:HB	5	0.34
(1,1783)	1:116:A:ALA:HB3	1:140:A:VAL:HB	5	0.34
(1,1520)	1:179:A:GLN:HA	1:179:A:GLN:HG3	9	0.34
(1,1510)	1:111:A:VAL:HG11	1:112:A:PRO:HD3	11	0.34
(1,1510)	1:111:A:VAL:HG12	1:112:A:PRO:HD3	11	0.34
(1,1510)	1:111:A:VAL:HG13	1:112:A:PRO:HD3	11	0.34
(1,1372)	1:177:A:VAL:HG21	1:118:A:ARG:HD3	7	0.34
(1,1372)	1:177:A:VAL:HG22	1:118:A:ARG:HD3	7	0.34
(1,1372)	1:177:A:VAL:HG23	1:118:A:ARG:HD3	7	0.34
(1,1334)	1:57:A:LYS:HE3	1:57:A:LYS:HG3	6	0.34
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	2	0.34
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	2	0.34
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	2	0.34
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	2	0.34
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	2	0.34
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	2	0.34
(1,1079)	1:59:A:ALA:HB1	1:70:A:MET:H	6	0.34
(1,1079)	1:59:A:ALA:HB2	1:70:A:MET:H	6	0.34
(1,1079)	1:59:A:ALA:HB3	1:70:A:MET:H	6	0.34
(1,1070)	1:178:A:LYS:HG2	1:178:A:LYS:HA	11	0.34
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	3	0.34
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	3	0.34
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	3	0.34
(1,547)	1:97:A:PHE:H	1:92:A:LYS:HA	4	0.34
(1,539)	1:179:A:GLN:H	1:176:A:GLN:HA	10	0.34
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	11	0.34
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	11	0.34
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	11	0.34
(1,221)	1:91:A:LEU:H	1:91:A:LEU:HG	6	0.34
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	4	0.33
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	4	0.33
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	4	0.33
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	4	0.33
(2,12)	1:71:A:VAL:H	1:73:A:ILE:H	11	0.33
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	6	0.33
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	5	0.33
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG21	11	0.33
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG22	11	0.33
(1,1760)	1:57:A:LYS:HE2	1:72:A:VAL:HG23	11	0.33
(1,1758)	1:57:A:LYS:HE2	1:57:A:LYS:HG2	8	0.33
(1,1749)	1:104:A:LYS:HE2	1:157:A:ILE:HG21	12	0.33
(1,1717)	1:50:A:ARG:HD2	1:50:A:ARG:HB3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	4	0.33
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	4	0.33
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	4	0.33
(1,1496)	1:87:A:ILE:HB	1:84:A:GLN:HA	5	0.33
(1,1466)	1:131:A:GLN:HG3	1:131:A:GLN:HA	2	0.33
(1,1334)	1:57:A:LYS:HE3	1:57:A:LYS:HG3	3	0.33
(1,1203)	1:110:A:ARG:HD3	1:151:A:GLN:HB2	4	0.33
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	10	0.33
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	4	0.33
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	4	0.33
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	4	0.33
(1,1012)	1:151:A:GLN:HG3	1:113:A:ALA:H	2	0.33
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	9	0.33
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	9	0.33
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	9	0.33
(1,949)	1:94:A:GLU:HG2	1:96:A:PHE:HZ	6	0.33
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	6	0.33
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB3	11	0.33
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	3	0.33
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	4	0.33
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	12	0.33
(1,376)	1:57:A:LYS:H	1:57:A:LYS:HD2	1	0.33
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG21	4	0.32
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG22	4	0.32
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG23	4	0.32
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG11	9	0.32
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG12	9	0.32
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG13	9	0.32
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG11	9	0.32
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG12	9	0.32
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG13	9	0.32
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG11	9	0.32
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG12	9	0.32
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG13	9	0.32
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	1	0.32
(1,1686)	1:113:A:ALA:HB2	1:150:A:GLU:HB3	4	0.32
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	4	0.32
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	4	0.32
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	4	0.32
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	4	0.32
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	4	0.32
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	4	0.32
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	4	0.32
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	4	0.32
(1,1621)	1:151:A:GLN:HA	1:112:A:PRO:HA	8	0.32
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	10	0.32
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	10	0.32
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	10	0.32
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	10	0.32
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	10	0.32
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	10	0.32
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	10	0.32
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	10	0.32
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	10	0.32
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB1	1	0.32
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB2	1	0.32
(1,1586)	1:177:A:VAL:HG21	1:115:A:ALA:HB3	1	0.32
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB1	1	0.32
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB2	1	0.32
(1,1586)	1:177:A:VAL:HG22	1:115:A:ALA:HB3	1	0.32
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB1	1	0.32
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB2	1	0.32
(1,1586)	1:177:A:VAL:HG23	1:115:A:ALA:HB3	1	0.32
(1,1496)	1:87:A:ILE:HB	1:84:A:GLN:HA	6	0.32
(1,1368)	1:48:A:LEU:HD21	1:83:A:ALA:HA	7	0.32
(1,1368)	1:48:A:LEU:HD22	1:83:A:ALA:HA	7	0.32
(1,1368)	1:48:A:LEU:HD23	1:83:A:ALA:HA	7	0.32
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	7	0.32
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	7	0.32
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	7	0.32
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	1	0.32
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG21	1	0.32
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG22	1	0.32
(1,1172)	1:116:A:ALA:HA	1:111:A:VAL:HG23	1	0.32
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE1	12	0.32
(1,1122)	1:91:A:LEU:HD21	1:96:A:PHE:HE2	12	0.32
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE1	12	0.32
(1,1122)	1:91:A:LEU:HD22	1:96:A:PHE:HE2	12	0.32
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE1	12	0.32
(1,1122)	1:91:A:LEU:HD23	1:96:A:PHE:HE2	12	0.32
(1,693)	1:126:A:THR:HB	1:126:A:THR:HA	8	0.32
(1,693)	1:126:A:THR:HB	1:126:A:THR:HA	9	0.32
(1,693)	1:126:A:THR:HB	1:126:A:THR:HA	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:179:A:GLN:H	1:176:A:GLN:HA	9	0.32
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	1	0.32
(1,133)	1:101:A:GLU:H	1:101:A:GLU:HB2	9	0.32
(2,53)	1:58:A:ILE:HD11	1:71:A:VAL:HA	4	0.31
(2,53)	1:58:A:ILE:HD12	1:71:A:VAL:HA	4	0.31
(2,53)	1:58:A:ILE:HD13	1:71:A:VAL:HA	4	0.31
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	6	0.31
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	6	0.31
(1,1906)	1:142:A:ARG:HA	1:142:A:ARG:HD2	10	0.31
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	3	0.31
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG11	2	0.31
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG12	2	0.31
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG13	2	0.31
(1,1708)	1:48:A:LEU:HD11	1:48:A:LEU:HB2	10	0.31
(1,1708)	1:48:A:LEU:HD12	1:48:A:LEU:HB2	10	0.31
(1,1708)	1:48:A:LEU:HD13	1:48:A:LEU:HB2	10	0.31
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	7	0.31
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	7	0.31
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	7	0.31
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	7	0.31
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	7	0.31
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	7	0.31
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	7	0.31
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	7	0.31
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	7	0.31
(1,1412)	1:171:A:ARG:HB3	1:168:A:ARG:HA	1	0.31
(1,1411)	1:122:A:LYS:HG2	1:122:A:LYS:HA	5	0.31
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	6	0.31
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	6	0.31
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	6	0.31
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	4	0.31
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	8	0.31
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	11	0.31
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	8	0.31
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	8	0.31
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	8	0.31
(1,693)	1:126:A:THR:HB	1:126:A:THR:HA	10	0.31
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD11	11	0.31
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD12	11	0.31
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD13	11	0.31
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	3	0.31
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB3	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB3	5	0.31
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	3	0.3
(1,2051)	1:177:A:VAL:HG21	2:2:B:C:H1'	8	0.3
(1,2051)	1:177:A:VAL:HG22	2:2:B:C:H1'	8	0.3
(1,2051)	1:177:A:VAL:HG23	2:2:B:C:H1'	8	0.3
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	2	0.3
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	2	0.3
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG21	10	0.3
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG22	10	0.3
(1,1920)	1:69:A:ARG:HA	1:34:A:VAL:HG23	10	0.3
(1,1840)	1:27:A:VAL:HG11	1:107:A:THR:HA	10	0.3
(1,1840)	1:27:A:VAL:HG12	1:107:A:THR:HA	10	0.3
(1,1840)	1:27:A:VAL:HG13	1:107:A:THR:HA	10	0.3
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	10	0.3
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	10	0.3
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	10	0.3
(1,1756)	1:57:A:LYS:HE3	1:57:A:LYS:HB2	9	0.3
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	10	0.3
(1,1717)	1:50:A:ARG:HD2	1:50:A:ARG:HB3	12	0.3
(1,1654)	1:105:A:LEU:HD21	1:91:A:LEU:HG	11	0.3
(1,1654)	1:105:A:LEU:HD22	1:91:A:LEU:HG	11	0.3
(1,1654)	1:105:A:LEU:HD23	1:91:A:LEU:HG	11	0.3
(1,1466)	1:131:A:GLN:HG3	1:131:A:GLN:HA	9	0.3
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	11	0.3
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	11	0.3
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	11	0.3
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	3	0.3
(1,483)	1:143:A:ASP:H	1:142:A:ARG:HG2	2	0.3
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	11	0.29
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	11	0.29
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	11	0.29
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	8	0.29
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	1	0.29
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	10	0.29
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	10	0.29
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	10	0.29
(1,1818)	1:90:A:LYS:HE3	1:94:A:GLU:HG2	3	0.29
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	7	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG11	11	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG12	11	0.29
(1,1759)	1:57:A:LYS:HE2	1:72:A:VAL:HG13	11	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	1	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	1	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	3	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	3	0.29
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	3	0.29
(1,1708)	1:48:A:LEU:HD11	1:48:A:LEU:HB2	7	0.29
(1,1708)	1:48:A:LEU:HD12	1:48:A:LEU:HB2	7	0.29
(1,1708)	1:48:A:LEU:HD13	1:48:A:LEU:HB2	7	0.29
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	11	0.29
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	11	0.29
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	11	0.29
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	11	0.29
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	11	0.29
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	11	0.29
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	11	0.29
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	11	0.29
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	11	0.29
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	2	0.29
(1,1607)	1:116:A:ALA:HB1	1:152:A:VAL:HG21	12	0.29
(1,1607)	1:116:A:ALA:HB1	1:152:A:VAL:HG22	12	0.29
(1,1607)	1:116:A:ALA:HB1	1:152:A:VAL:HG23	12	0.29
(1,1607)	1:116:A:ALA:HB2	1:152:A:VAL:HG21	12	0.29
(1,1607)	1:116:A:ALA:HB2	1:152:A:VAL:HG22	12	0.29
(1,1607)	1:116:A:ALA:HB2	1:152:A:VAL:HG23	12	0.29
(1,1607)	1:116:A:ALA:HB3	1:152:A:VAL:HG21	12	0.29
(1,1607)	1:116:A:ALA:HB3	1:152:A:VAL:HG22	12	0.29
(1,1607)	1:116:A:ALA:HB3	1:152:A:VAL:HG23	12	0.29
(1,1495)	1:177:A:VAL:HG11	1:177:A:VAL:HA	11	0.29
(1,1495)	1:177:A:VAL:HG12	1:177:A:VAL:HA	11	0.29
(1,1495)	1:177:A:VAL:HG13	1:177:A:VAL:HA	11	0.29
(1,1378)	1:142:A:ARG:HB2	1:141:A:PRO:HB3	12	0.29
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	1	0.29
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	2	0.29
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	10	0.29
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	10	0.29
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	10	0.29
(1,1309)	1:91:A:LEU:HD21	1:96:A:PHE:HB2	1	0.29
(1,1309)	1:91:A:LEU:HD22	1:96:A:PHE:HB2	1	0.29
(1,1309)	1:91:A:LEU:HD23	1:96:A:PHE:HB2	1	0.29
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	3	0.29
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	3	0.29
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:102:A:GLU:HB2	1:103:A:VAL:H	5	0.29
(1,588)	1:58:A:ILE:HB	1:59:A:ALA:H	10	0.29
(1,558)	1:83:A:ALA:H	1:86:A:ARG:HB2	11	0.29
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB3	4	0.29
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	5	0.29
(1,365)	1:102:A:GLU:H	1:102:A:GLU:HB3	11	0.29
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	1	0.28
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	5	0.28
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	5	0.28
(1,1912)	1:156:A:ILE:HG21	1:166:A:ALA:HA	7	0.28
(1,1912)	1:156:A:ILE:HG22	1:166:A:ALA:HA	7	0.28
(1,1912)	1:156:A:ILE:HG23	1:166:A:ALA:HA	7	0.28
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	2	0.28
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	2	0.28
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	2	0.28
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	11	0.28
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	7	0.28
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	9	0.28
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	9	0.28
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	9	0.28
(1,1495)	1:177:A:VAL:HG11	1:177:A:VAL:HA	8	0.28
(1,1495)	1:177:A:VAL:HG12	1:177:A:VAL:HA	8	0.28
(1,1495)	1:177:A:VAL:HG13	1:177:A:VAL:HA	8	0.28
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	2	0.28
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	2	0.28
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	2	0.28
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	8	0.28
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	5	0.28
(1,1044)	1:99:A:PRO:HD3	1:99:A:PRO:HB2	3	0.28
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	8	0.28
(1,352)	1:57:A:LYS:H	1:57:A:LYS:HG2	11	0.28
(1,218)	1:96:A:PHE:H	1:94:A:GLU:HB2	10	0.28
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	4	0.27
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	4	0.27
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	4	0.27
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	4	0.27
(1,1708)	1:48:A:LEU:HD11	1:48:A:LEU:HB2	4	0.27
(1,1708)	1:48:A:LEU:HD12	1:48:A:LEU:HB2	4	0.27
(1,1708)	1:48:A:LEU:HD13	1:48:A:LEU:HB2	4	0.27
(1,1478)	1:176:A:GLN:HG2	1:176:A:GLN:HA	3	0.27
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	4	0.27
(1,1275)	1:92:A:LYS:HD2	1:92:A:LYS:HA	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG2	6	0.27
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG2	6	0.27
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG2	6	0.27
(1,1185)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	3	0.27
(1,1185)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	3	0.27
(1,1185)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	3	0.27
(1,1173)	1:116:A:ALA:HB1	1:119:A:VAL:HB	2	0.27
(1,1173)	1:116:A:ALA:HB2	1:119:A:VAL:HB	2	0.27
(1,1173)	1:116:A:ALA:HB3	1:119:A:VAL:HB	2	0.27
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	1	0.27
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	6	0.27
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	9	0.27
(1,1044)	1:99:A:PRO:HD3	1:99:A:PRO:HB2	10	0.27
(1,900)	1:58:A:ILE:HB	1:58:A:ILE:HD11	11	0.27
(1,900)	1:58:A:ILE:HB	1:58:A:ILE:HD12	11	0.27
(1,900)	1:58:A:ILE:HB	1:58:A:ILE:HD13	11	0.27
(1,669)	1:146:A:PRO:HD2	1:145:A:THR:HA	3	0.27
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	9	0.27
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	10	0.26
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	10	0.26
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	10	0.26
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	11	0.26
(1,2050)	1:177:A:VAL:HG11	2:2:B:C:H1'	11	0.26
(1,2050)	1:177:A:VAL:HG12	2:2:B:C:H1'	11	0.26
(1,2050)	1:177:A:VAL:HG13	2:2:B:C:H1'	11	0.26
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG21	12	0.26
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG22	12	0.26
(1,1977)	1:97:A:PHE:HE1	1:103:A:VAL:HG23	12	0.26
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG21	12	0.26
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG22	12	0.26
(1,1977)	1:97:A:PHE:HE2	1:103:A:VAL:HG23	12	0.26
(1,1924)	1:151:A:GLN:HG3	1:112:A:PRO:HA	5	0.26
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG21	8	0.26
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG22	8	0.26
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG23	8	0.26
(1,1859)	1:63:A:THR:HB	1:64:A:PRO:HB3	5	0.26
(1,1840)	1:27:A:VAL:HG11	1:107:A:THR:HA	8	0.26
(1,1840)	1:27:A:VAL:HG12	1:107:A:THR:HA	8	0.26
(1,1840)	1:27:A:VAL:HG13	1:107:A:THR:HA	8	0.26
(1,1686)	1:113:A:ALA:HB3	1:150:A:GLU:HB3	3	0.26
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	1	0.26
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	1	0.26
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	1	0.26
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	1	0.26
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	1	0.26
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	1	0.26
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	1	0.26
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	1	0.26
(1,1663)	1:105:A:LEU:HD11	1:88:A:TYR:HA	2	0.26
(1,1663)	1:105:A:LEU:HD12	1:88:A:TYR:HA	2	0.26
(1,1663)	1:105:A:LEU:HD13	1:88:A:TYR:HA	2	0.26
(1,1621)	1:151:A:GLN:HA	1:112:A:PRO:HA	9	0.26
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	3	0.26
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	3	0.26
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	3	0.26
(1,1443)	1:58:A:ILE:HG21	1:58:A:ILE:HA	10	0.26
(1,1443)	1:58:A:ILE:HG22	1:58:A:ILE:HA	10	0.26
(1,1443)	1:58:A:ILE:HG23	1:58:A:ILE:HA	10	0.26
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	8	0.26
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	8	0.26
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	6	0.26
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	6	0.26
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	6	0.26
(1,1378)	1:142:A:ARG:HB3	1:141:A:PRO:HB3	7	0.26
(1,1361)	1:27:A:VAL:HG11	1:26:A:HIS:H	7	0.26
(1,1361)	1:27:A:VAL:HG12	1:26:A:HIS:H	7	0.26
(1,1361)	1:27:A:VAL:HG13	1:26:A:HIS:H	7	0.26
(1,1257)	1:170:A:ILE:HD11	1:109:A:ILE:HG12	4	0.26
(1,1257)	1:170:A:ILE:HD12	1:109:A:ILE:HG12	4	0.26
(1,1257)	1:170:A:ILE:HD13	1:109:A:ILE:HG12	4	0.26
(1,1191)	1:105:A:LEU:HD11	1:104:A:LYS:HD2	8	0.26
(1,1191)	1:105:A:LEU:HD12	1:104:A:LYS:HD2	8	0.26
(1,1191)	1:105:A:LEU:HD13	1:104:A:LYS:HD2	8	0.26
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG2	6	0.26
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	1	0.26
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	7	0.26
(1,979)	1:105:A:LEU:HG	1:91:A:LEU:HG	12	0.26
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	11	0.26
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	11	0.26
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	11	0.26
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	9	0.26
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	9	0.26
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	10	0.26
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	10	0.26
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	10	0.26
(1,598)	1:102:A:GLU:HB2	1:103:A:VAL:H	3	0.26
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	11	0.26
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD11	8	0.26
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD12	8	0.26
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD13	8	0.26
(1,482)	1:143:A:ASP:H	1:142:A:ARG:HB2	1	0.26
(1,452)	1:98:A:GLY:H	1:99:A:PRO:HB2	7	0.26
(1,407)	1:18:A:MET:H	1:17:A:PHE:HA	11	0.26
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG21	7	0.26
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG22	7	0.26
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG23	7	0.26
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	9	0.26
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	10	0.26
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	11	0.26
(1,152)	1:24:A:THR:H	1:23:A:GLU:HG2	2	0.26
(1,34)	1:57:A:LYS:H	1:72:A:VAL:H	11	0.26
(2,102)	1:142:A:ARG:NH1	2:5:B:A:OP1	5	0.25
(2,44)	1:56:A:ILE:HD11	1:87:A:ILE:HG13	11	0.25
(2,44)	1:56:A:ILE:HD12	1:87:A:ILE:HG13	11	0.25
(2,44)	1:56:A:ILE:HD13	1:87:A:ILE:HG13	11	0.25
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	8	0.25
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	4	0.25
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	6	0.25
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	9	0.25
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	3	0.25
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	3	0.25
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	3	0.25
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB3	12	0.25
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB3	12	0.25
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB3	12	0.25
(1,1443)	1:58:A:ILE:HG21	1:58:A:ILE:HA	9	0.25
(1,1443)	1:58:A:ILE:HG22	1:58:A:ILE:HA	9	0.25
(1,1443)	1:58:A:ILE:HG23	1:58:A:ILE:HA	9	0.25
(1,1439)	1:105:A:LEU:HD11	1:105:A:LEU:HA	12	0.25
(1,1439)	1:105:A:LEU:HD12	1:105:A:LEU:HA	12	0.25
(1,1439)	1:105:A:LEU:HD13	1:105:A:LEU:HA	12	0.25
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	6	0.25
(1,1198)	1:114:A:SER:HA	1:150:A:GLU:HB3	12	0.25
(1,1137)	1:155:A:LYS:HB2	1:157:A:ILE:HD12	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	12	0.25
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	10	0.25
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	10	0.25
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	10	0.25
(1,445)	1:68:A:VAL:H	1:31:A:ALA:HB1	5	0.25
(1,445)	1:68:A:VAL:H	1:31:A:ALA:HB2	5	0.25
(1,445)	1:68:A:VAL:H	1:31:A:ALA:HB3	5	0.25
(1,442)	1:91:A:LEU:H	1:90:A:LYS:HD2	6	0.25
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	8	0.25
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	5	0.24
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	5	0.24
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	5	0.24
(2,45)	1:34:A:VAL:HG11	1:58:A:ILE:HA	11	0.24
(2,45)	1:34:A:VAL:HG12	1:58:A:ILE:HA	11	0.24
(2,45)	1:34:A:VAL:HG13	1:58:A:ILE:HA	11	0.24
(2,43)	1:157:A:ILE:HD11	1:105:A:LEU:HB2	5	0.24
(2,43)	1:157:A:ILE:HD12	1:105:A:LEU:HB2	5	0.24
(2,43)	1:157:A:ILE:HD13	1:105:A:LEU:HB2	5	0.24
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	4	0.24
(1,2050)	1:177:A:VAL:HG11	2:2:B:C:H1'	8	0.24
(1,2050)	1:177:A:VAL:HG12	2:2:B:C:H1'	8	0.24
(1,2050)	1:177:A:VAL:HG13	2:2:B:C:H1'	8	0.24
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG21	1	0.24
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG22	1	0.24
(1,1874)	1:57:A:LYS:HD2	1:72:A:VAL:HG23	1	0.24
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG11	5	0.24
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG12	5	0.24
(1,1811)	1:174:A:LEU:HD21	1:177:A:VAL:HG13	5	0.24
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG11	5	0.24
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG12	5	0.24
(1,1811)	1:174:A:LEU:HD22	1:177:A:VAL:HG13	5	0.24
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG11	5	0.24
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG12	5	0.24
(1,1811)	1:174:A:LEU:HD23	1:177:A:VAL:HG13	5	0.24
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	5	0.24
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	5	0.24
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	5	0.24
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	5	0.24
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	5	0.24
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	5	0.24
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	5	0.24
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	5	0.24
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	5	0.24
(1,1497)	1:105:A:LEU:HD21	1:88:A:TYR:HA	8	0.24
(1,1497)	1:105:A:LEU:HD22	1:88:A:TYR:HA	8	0.24
(1,1497)	1:105:A:LEU:HD23	1:88:A:TYR:HA	8	0.24
(1,1471)	1:86:A:ARG:HD3	1:86:A:ARG:HA	8	0.24
(1,1469)	1:32:A:GLN:HG3	1:32:A:GLN:HA	8	0.24
(1,1445)	1:146:A:PRO:HD3	1:145:A:THR:HA	3	0.24
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	9	0.24
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	9	0.24
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	9	0.24
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	3	0.24
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	5	0.24
(1,1045)	1:99:A:PRO:HD2	1:99:A:PRO:HB3	2	0.24
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	7	0.24
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	7	0.24
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	7	0.24
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	10	0.24
(1,516)	1:100:A:LYS:H	1:99:A:PRO:HB2	8	0.24
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	6	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG21	1	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG22	1	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG23	1	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG21	5	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG22	5	0.24
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG23	5	0.24
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG21	6	0.24
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG22	6	0.24
(1,353)	1:57:A:LYS:H	1:58:A:ILE:HG23	6	0.24
(1,352)	1:57:A:LYS:H	1:57:A:LYS:HG2	6	0.24
(2,100)	1:143:A:ASP:OD1	2:4:B:G:H22	7	0.23
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	11	0.23
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	11	0.23
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG21	3	0.23
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG22	3	0.23
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG23	3	0.23
(1,1851)	1:153:A:ILE:HG21	1:141:A:PRO:HD3	11	0.23
(1,1851)	1:153:A:ILE:HG22	1:141:A:PRO:HD3	11	0.23
(1,1851)	1:153:A:ILE:HG23	1:141:A:PRO:HD3	11	0.23
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG11	11	0.23
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG12	11	0.23
(1,1739)	1:92:A:LYS:HE2	1:103:A:VAL:HG13	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD11	9	0.23
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD12	9	0.23
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD13	9	0.23
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD11	9	0.23
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD12	9	0.23
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD13	9	0.23
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD11	9	0.23
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD12	9	0.23
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD13	9	0.23
(1,1668)	1:32:A:GLN:HA	1:32:A:GLN:HB2	10	0.23
(1,1668)	1:32:A:GLN:HA	1:32:A:GLN:HB2	11	0.23
(1,1654)	1:105:A:LEU:HD21	1:91:A:LEU:HG	8	0.23
(1,1654)	1:105:A:LEU:HD22	1:91:A:LEU:HG	8	0.23
(1,1654)	1:105:A:LEU:HD23	1:91:A:LEU:HG	8	0.23
(1,1518)	1:103:A:VAL:HG11	1:103:A:VAL:HA	10	0.23
(1,1518)	1:103:A:VAL:HG12	1:103:A:VAL:HA	10	0.23
(1,1518)	1:103:A:VAL:HG13	1:103:A:VAL:HA	10	0.23
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	10	0.23
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	11	0.23
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	12	0.23
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG21	8	0.23
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG22	8	0.23
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG23	8	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG21	8	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG22	8	0.23
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG23	8	0.23
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG21	8	0.23
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG22	8	0.23
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG23	8	0.23
(1,830)	1:171:A:ARG:HA	1:174:A:LEU:HB3	10	0.23
(1,631)	1:176:A:GLN:HG3	1:176:A:GLN:H	3	0.23
(1,481)	1:158:A:GLY:H	1:136:A:ALA:HA	4	0.23
(1,337)	1:149:A:ASN:HD21	1:149:A:ASN:H	9	0.23
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	4	0.23
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	11	0.22
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	3	0.22
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	6	0.22
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	10	0.22
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	3	0.22
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	3	0.22
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD21	12	0.22
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD22	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:96:A:PHE:HD1	1:91:A:LEU:HD23	12	0.22
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD21	12	0.22
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD22	12	0.22
(1,1950)	1:96:A:PHE:HD2	1:91:A:LEU:HD23	12	0.22
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	1	0.22
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	1	0.22
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	1	0.22
(1,1791)	1:104:A:LYS:HE2	1:104:A:LYS:HB3	10	0.22
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG11	11	0.22
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG12	11	0.22
(1,1784)	1:116:A:ALA:HB1	1:152:A:VAL:HG13	11	0.22
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG11	11	0.22
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG12	11	0.22
(1,1784)	1:116:A:ALA:HB2	1:152:A:VAL:HG13	11	0.22
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG11	11	0.22
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG12	11	0.22
(1,1784)	1:116:A:ALA:HB3	1:152:A:VAL:HG13	11	0.22
(1,1783)	1:116:A:ALA:HB1	1:140:A:VAL:HB	9	0.22
(1,1783)	1:116:A:ALA:HB2	1:140:A:VAL:HB	9	0.22
(1,1783)	1:116:A:ALA:HB3	1:140:A:VAL:HB	9	0.22
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	12	0.22
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	12	0.22
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	12	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD11	6	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD12	6	0.22
(1,1709)	1:91:A:LEU:HD21	1:105:A:LEU:HD13	6	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD11	6	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD12	6	0.22
(1,1709)	1:91:A:LEU:HD22	1:105:A:LEU:HD13	6	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD11	6	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD12	6	0.22
(1,1709)	1:91:A:LEU:HD23	1:105:A:LEU:HD13	6	0.22
(1,1672)	1:115:A:ALA:HB1	1:112:A:PRO:HG2	8	0.22
(1,1672)	1:115:A:ALA:HB2	1:112:A:PRO:HG2	8	0.22
(1,1672)	1:115:A:ALA:HB3	1:112:A:PRO:HG2	8	0.22
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	3	0.22
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	3	0.22
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	3	0.22
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	3	0.22
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	3	0.22
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	3	0.22
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	3	0.22
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	3	0.22
(1,1668)	1:32:A:GLN:HA	1:32:A:GLN:HB2	9	0.22
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	2	0.22
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	10	0.22
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	10	0.22
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	10	0.22
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	2	0.22
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	5	0.22
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	9	0.22
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD3	10	0.22
(1,1309)	1:91:A:LEU:HD21	1:96:A:PHE:HB2	4	0.22
(1,1309)	1:91:A:LEU:HD22	1:96:A:PHE:HB2	4	0.22
(1,1309)	1:91:A:LEU:HD23	1:96:A:PHE:HB2	4	0.22
(1,1220)	1:146:A:PRO:HD2	1:144:A:GLN:HG2	6	0.22
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	11	0.22
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	11	0.22
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	11	0.22
(1,661)	1:174:A:LEU:HD11	1:111:A:VAL:HA	1	0.22
(1,661)	1:174:A:LEU:HD12	1:111:A:VAL:HA	1	0.22
(1,661)	1:174:A:LEU:HD13	1:111:A:VAL:HA	1	0.22
(1,631)	1:176:A:GLN:HG3	1:176:A:GLN:H	4	0.22
(1,483)	1:143:A:ASP:H	1:142:A:ARG:HG2	4	0.22
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG11	3	0.22
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG12	3	0.22
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG13	3	0.22
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG21	6	0.22
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG22	6	0.22
(1,393)	1:170:A:ILE:H	1:170:A:ILE:HG23	6	0.22
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	1	0.22
(1,221)	1:91:A:LEU:H	1:91:A:LEU:HG	12	0.22
(1,34)	1:57:A:LYS:H	1:72:A:VAL:H	6	0.22
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	7	0.21
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	1	0.21
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	3	0.21
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	3	0.21
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	3	0.21
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	9	0.21
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	9	0.21
(1,1924)	1:151:A:GLN:HG3	1:112:A:PRO:HA	3	0.21
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	3	0.21
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	9	0.21
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	9	0.21
(1,1717)	1:50:A:ARG:HD3	1:50:A:ARG:HB2	10	0.21
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	7	0.21
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	7	0.21
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	7	0.21
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	7	0.21
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	7	0.21
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	7	0.21
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	7	0.21
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	7	0.21
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	7	0.21
(1,1496)	1:87:A:ILE:HB	1:84:A:GLN:HA	2	0.21
(1,1443)	1:58:A:ILE:HG21	1:58:A:ILE:HA	8	0.21
(1,1443)	1:58:A:ILE:HG22	1:58:A:ILE:HA	8	0.21
(1,1443)	1:58:A:ILE:HG23	1:58:A:ILE:HA	8	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	1	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	1	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	1	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	8	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	8	0.21
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	8	0.21
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	7	0.21
(1,1206)	1:56:A:ILE:HD11	1:71:A:VAL:H	10	0.21
(1,1206)	1:56:A:ILE:HD12	1:71:A:VAL:H	10	0.21
(1,1206)	1:56:A:ILE:HD13	1:71:A:VAL:H	10	0.21
(1,928)	1:47:A:GLN:HB2	1:47:A:GLN:HG3	3	0.21
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	9	0.21
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD11	6	0.21
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD12	6	0.21
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD13	6	0.21
(1,547)	1:97:A:PHE:H	1:92:A:LYS:HA	10	0.21
(1,419)	1:153:A:ILE:H	1:152:A:VAL:HB	12	0.21
(1,302)	1:63:A:THR:H	1:63:A:THR:HG21	5	0.21
(1,302)	1:63:A:THR:H	1:63:A:THR:HG22	5	0.21
(1,302)	1:63:A:THR:H	1:63:A:THR:HG23	5	0.21
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	5	0.21
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	8	0.2
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	8	0.2
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	8	0.2
(2,45)	1:34:A:VAL:HG11	1:58:A:ILE:HA	9	0.2
(2,45)	1:34:A:VAL:HG12	1:58:A:ILE:HA	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:34:A:VAL:HG13	1:58:A:ILE:HA	9	0.2
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	9	0.2
(1,1851)	1:153:A:ILE:HG21	1:141:A:PRO:HD3	1	0.2
(1,1851)	1:153:A:ILE:HG22	1:141:A:PRO:HD3	1	0.2
(1,1851)	1:153:A:ILE:HG23	1:141:A:PRO:HD3	1	0.2
(1,1791)	1:104:A:LYS:HE3	1:104:A:LYS:HB3	9	0.2
(1,1732)	1:130:A:LEU:HD11	1:130:A:LEU:HB2	3	0.2
(1,1732)	1:130:A:LEU:HD12	1:130:A:LEU:HB2	3	0.2
(1,1732)	1:130:A:LEU:HD13	1:130:A:LEU:HB2	3	0.2
(1,1716)	1:67:A:LYS:HG3	1:67:A:LYS:HA	1	0.2
(1,1716)	1:67:A:LYS:HG3	1:67:A:LYS:HA	4	0.2
(1,1668)	1:32:A:GLN:HA	1:32:A:GLN:HB2	12	0.2
(1,1654)	1:105:A:LEU:HD21	1:91:A:LEU:HG	10	0.2
(1,1654)	1:105:A:LEU:HD22	1:91:A:LEU:HG	10	0.2
(1,1654)	1:105:A:LEU:HD23	1:91:A:LEU:HG	10	0.2
(1,1445)	1:146:A:PRO:HD3	1:145:A:THR:HA	5	0.2
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	9	0.2
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	9	0.2
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	9	0.2
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	7	0.2
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	7	0.2
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	7	0.2
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	11	0.2
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	11	0.2
(1,1337)	1:90:A:LYS:HB3	1:90:A:LYS:HE2	5	0.2
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	6	0.2
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	8	0.2
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	1	0.2
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	4	0.2
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	4	0.2
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	7	0.2
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	9	0.2
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	12	0.2
(1,997)	1:136:A:ALA:HB1	1:158:A:GLY:HA2	8	0.2
(1,997)	1:136:A:ALA:HB2	1:158:A:GLY:HA2	8	0.2
(1,997)	1:136:A:ALA:HB3	1:158:A:GLY:HA2	8	0.2
(1,928)	1:47:A:GLN:HB2	1:47:A:GLN:HG3	12	0.2
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG21	10	0.2
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG22	10	0.2
(1,889)	1:116:A:ALA:HB1	1:140:A:VAL:HG23	10	0.2
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG21	10	0.2
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG22	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:116:A:ALA:HB2	1:140:A:VAL:HG23	10	0.2
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG21	10	0.2
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG22	10	0.2
(1,889)	1:116:A:ALA:HB3	1:140:A:VAL:HG23	10	0.2
(1,830)	1:171:A:ARG:HA	1:174:A:LEU:HB3	11	0.2
(1,817)	1:170:A:ILE:HD11	1:170:A:ILE:HB	2	0.2
(1,817)	1:170:A:ILE:HD12	1:170:A:ILE:HB	2	0.2
(1,817)	1:170:A:ILE:HD13	1:170:A:ILE:HB	2	0.2
(1,481)	1:158:A:GLY:H	1:136:A:ALA:HA	7	0.2
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	6	0.2
(1,151)	1:22:A:GLN:H	1:22:A:GLN:HG2	5	0.2
(2,69)	1:93:A:GLU:HB3	1:94:A:GLU:HB2	7	0.19
(2,43)	1:157:A:ILE:HD11	1:105:A:LEU:HB2	2	0.19
(2,43)	1:157:A:ILE:HD12	1:105:A:LEU:HB2	2	0.19
(2,43)	1:157:A:ILE:HD13	1:105:A:LEU:HB2	2	0.19
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	8	0.19
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	8	0.19
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG21	12	0.19
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG22	12	0.19
(1,1928)	1:138:A:VAL:HB	1:127:A:VAL:HG23	12	0.19
(1,1912)	1:156:A:ILE:HG21	1:166:A:ALA:HA	1	0.19
(1,1912)	1:156:A:ILE:HG22	1:166:A:ALA:HA	1	0.19
(1,1912)	1:156:A:ILE:HG23	1:166:A:ALA:HA	1	0.19
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	4	0.19
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	4	0.19
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	4	0.19
(1,1840)	1:27:A:VAL:HG11	1:107:A:THR:HA	11	0.19
(1,1840)	1:27:A:VAL:HG12	1:107:A:THR:HA	11	0.19
(1,1840)	1:27:A:VAL:HG13	1:107:A:THR:HA	11	0.19
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG21	12	0.19
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG22	12	0.19
(1,1806)	1:48:A:LEU:HB2	1:58:A:ILE:HG23	12	0.19
(1,1723)	1:71:A:VAL:HB	1:71:A:VAL:HA	2	0.19
(1,1563)	1:100:A:LYS:HA	1:100:A:LYS:HD2	7	0.19
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	5	0.19
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	9	0.19
(1,1344)	1:92:A:LYS:HD2	1:103:A:VAL:HG11	7	0.19
(1,1344)	1:92:A:LYS:HD2	1:103:A:VAL:HG12	7	0.19
(1,1344)	1:92:A:LYS:HD2	1:103:A:VAL:HG13	7	0.19
(1,1125)	1:128:A:ASN:HB2	1:125:A:LYS:HA	2	0.19
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	10	0.19
(1,1086)	1:146:A:PRO:HG3	1:145:A:THR:HA	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	2	0.19
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	2	0.19
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	2	0.19
(1,775)	1:150:A:GLU:HG3	1:150:A:GLU:HB2	9	0.19
(1,592)	1:58:A:ILE:HG21	1:58:A:ILE:H	6	0.19
(1,592)	1:58:A:ILE:HG22	1:58:A:ILE:H	6	0.19
(1,592)	1:58:A:ILE:HG23	1:58:A:ILE:H	6	0.19
(1,522)	1:65:A:ASP:H	1:64:A:PRO:HD2	5	0.19
(1,218)	1:96:A:PHE:H	1:94:A:GLU:HB2	5	0.19
(2,80)	1:118:A:ARG:HD2	1:173:A:ILE:HD11	7	0.18
(2,80)	1:118:A:ARG:HD2	1:173:A:ILE:HD12	7	0.18
(2,80)	1:118:A:ARG:HD2	1:173:A:ILE:HD13	7	0.18
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	8	0.18
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	8	0.18
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	9	0.18
(1,1966)	1:108:A:HIS:HD2	1:155:A:LYS:HG3	11	0.18
(1,1961)	1:97:A:PHE:HD1	1:101:A:GLU:HG2	12	0.18
(1,1961)	1:97:A:PHE:HD2	1:101:A:GLU:HG2	12	0.18
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG21	1	0.18
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG22	1	0.18
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG23	1	0.18
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	12	0.18
(1,1767)	1:34:A:VAL:HG11	1:69:A:ARG:HB2	1	0.18
(1,1767)	1:34:A:VAL:HG12	1:69:A:ARG:HB2	1	0.18
(1,1767)	1:34:A:VAL:HG13	1:69:A:ARG:HB2	1	0.18
(1,1732)	1:130:A:LEU:HD11	1:130:A:LEU:HB2	12	0.18
(1,1732)	1:130:A:LEU:HD12	1:130:A:LEU:HB2	12	0.18
(1,1732)	1:130:A:LEU:HD13	1:130:A:LEU:HB2	12	0.18
(1,1716)	1:67:A:LYS:HG3	1:67:A:LYS:HA	6	0.18
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	2	0.18
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	2	0.18
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	2	0.18
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	2	0.18
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	2	0.18
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	2	0.18
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	2	0.18
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	2	0.18
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	2	0.18
(1,1663)	1:105:A:LEU:HD11	1:88:A:TYR:HA	5	0.18
(1,1663)	1:105:A:LEU:HD12	1:88:A:TYR:HA	5	0.18
(1,1663)	1:105:A:LEU:HD13	1:88:A:TYR:HA	5	0.18
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	5	0.18
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	5	0.18
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	5	0.18
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	5	0.18
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	5	0.18
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	5	0.18
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	5	0.18
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	5	0.18
(1,1587)	1:104:A:LYS:HE2	1:104:A:LYS:HG2	1	0.18
(1,1587)	1:104:A:LYS:HE2	1:104:A:LYS:HG2	7	0.18
(1,1563)	1:100:A:LYS:HA	1:100:A:LYS:HD2	12	0.18
(1,1538)	1:99:A:PRO:HA	1:99:A:PRO:HG3	10	0.18
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	3	0.18
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	4	0.18
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG21	3	0.18
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG22	3	0.18
(1,1418)	1:104:A:LYS:HD2	1:157:A:ILE:HG23	3	0.18
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	4	0.18
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	4	0.18
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	4	0.18
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG11	3	0.18
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG12	3	0.18
(1,884)	1:26:A:HIS:HA	1:25:A:VAL:HG13	3	0.18
(1,599)	1:110:A:ARG:HG2	1:110:A:ARG:H	7	0.18
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD11	9	0.18
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD12	9	0.18
(1,555)	1:46:A:LYS:H	1:58:A:ILE:HD13	9	0.18
(1,533)	1:22:A:GLN:H	1:22:A:GLN:HG3	9	0.18
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG2	7	0.18
(1,444)	1:68:A:VAL:H	1:65:A:ASP:HA	5	0.18
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	11	0.18
(1,218)	1:96:A:PHE:H	1:94:A:GLU:HB2	8	0.18
(2,90)	1:88:A:TYR:HD1	1:159:A:HIS:HB3	5	0.17
(2,90)	1:88:A:TYR:HD2	1:159:A:HIS:HB3	5	0.17
(2,79)	1:111:A:VAL:HG21	1:119:A:VAL:HA	2	0.17
(2,79)	1:111:A:VAL:HG22	1:119:A:VAL:HA	2	0.17
(2,79)	1:111:A:VAL:HG23	1:119:A:VAL:HA	2	0.17
(2,49)	1:120:A:ILE:HG21	1:127:A:VAL:HB	9	0.17
(2,49)	1:120:A:ILE:HG22	1:127:A:VAL:HB	9	0.17
(2,49)	1:120:A:ILE:HG23	1:127:A:VAL:HB	9	0.17
(1,2088)	1:171:A:ARG:H	1:172:A:ASP:H	3	0.17
(1,2077)	1:176:A:GLN:HA	1:179:A:GLN:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	7	0.17
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	12	0.17
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	12	0.17
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	12	0.17
(1,1940)	1:28:A:PHE:HD1	1:106:A:GLU:HB2	5	0.17
(1,1940)	1:28:A:PHE:HD2	1:106:A:GLU:HB2	5	0.17
(1,1908)	1:18:A:MET:HA	1:19:A:PRO:HD2	1	0.17
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG21	9	0.17
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG22	9	0.17
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG23	9	0.17
(1,1884)	1:33:A:ALA:HA	1:96:A:PHE:HE1	8	0.17
(1,1884)	1:33:A:ALA:HA	1:96:A:PHE:HE2	8	0.17
(1,1722)	1:76:A:PRO:HB2	1:77:A:PRO:HG2	6	0.17
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD21	9	0.17
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD22	9	0.17
(1,1671)	1:103:A:VAL:HG21	1:105:A:LEU:HD23	9	0.17
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD21	9	0.17
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD22	9	0.17
(1,1671)	1:103:A:VAL:HG22	1:105:A:LEU:HD23	9	0.17
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD21	9	0.17
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD22	9	0.17
(1,1671)	1:103:A:VAL:HG23	1:105:A:LEU:HD23	9	0.17
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	9	0.17
(1,1538)	1:99:A:PRO:HA	1:99:A:PRO:HG3	3	0.17
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	10	0.17
(1,1520)	1:179:A:GLN:HA	1:179:A:GLN:HG3	7	0.17
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	5	0.17
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	5	0.17
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	5	0.17
(1,1412)	1:171:A:ARG:HB3	1:168:A:ARG:HA	2	0.17
(1,1354)	1:56:A:ILE:HD11	1:45:A:ILE:HG13	11	0.17
(1,1354)	1:56:A:ILE:HD12	1:45:A:ILE:HG13	11	0.17
(1,1354)	1:56:A:ILE:HD13	1:45:A:ILE:HG13	11	0.17
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	8	0.17
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	8	0.17
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	1	0.17
(1,1332)	1:118:A:ARG:HD3	1:177:A:VAL:HG11	11	0.17
(1,1332)	1:118:A:ARG:HD3	1:177:A:VAL:HG12	11	0.17
(1,1332)	1:118:A:ARG:HD3	1:177:A:VAL:HG13	11	0.17
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	1	0.17
(1,1331)	1:178:A:LYS:HG3	1:178:A:LYS:HD2	4	0.17
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	6	0.17
(1,1304)	1:177:A:VAL:HG11	1:115:A:ALA:HB1	8	0.17
(1,1304)	1:177:A:VAL:HG11	1:115:A:ALA:HB2	8	0.17
(1,1304)	1:177:A:VAL:HG11	1:115:A:ALA:HB3	8	0.17
(1,1304)	1:177:A:VAL:HG12	1:115:A:ALA:HB1	8	0.17
(1,1304)	1:177:A:VAL:HG12	1:115:A:ALA:HB2	8	0.17
(1,1304)	1:177:A:VAL:HG12	1:115:A:ALA:HB3	8	0.17
(1,1304)	1:177:A:VAL:HG13	1:115:A:ALA:HB1	8	0.17
(1,1304)	1:177:A:VAL:HG13	1:115:A:ALA:HB2	8	0.17
(1,1304)	1:177:A:VAL:HG13	1:115:A:ALA:HB3	8	0.17
(1,1299)	1:102:A:GLU:HG3	1:102:A:GLU:H	10	0.17
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	6	0.17
(1,1123)	1:86:A:ARG:HD2	1:86:A:ARG:HG2	7	0.17
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	1	0.17
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	3	0.17
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	8	0.17
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	1	0.17
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	1	0.17
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	1	0.17
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	5	0.17
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	5	0.17
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	5	0.17
(1,830)	1:171:A:ARG:HA	1:174:A:LEU:HB3	8	0.17
(1,723)	1:111:A:VAL:HB	1:112:A:PRO:HD2	12	0.17
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	6	0.17
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	7	0.17
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	11	0.17
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	7	0.17
(2,12)	1:71:A:VAL:H	1:73:A:ILE:H	6	0.16
(1,2082)	1:165:A:MET:H	1:166:A:ALA:H	4	0.16
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	10	0.16
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	5	0.16
(1,1980)	1:88:A:TYR:HE1	1:159:A:HIS:HA	12	0.16
(1,1980)	1:88:A:TYR:HE2	1:159:A:HIS:HA	12	0.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD11	5	0.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD12	5	0.16
(1,1958)	1:97:A:PHE:HD1	1:91:A:LEU:HD13	5	0.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD11	5	0.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD12	5	0.16
(1,1958)	1:97:A:PHE:HD2	1:91:A:LEU:HD13	5	0.16
(1,1945)	1:88:A:TYR:HD1	1:103:A:VAL:HB	12	0.16
(1,1945)	1:88:A:TYR:HD2	1:103:A:VAL:HB	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG21	11	0.16
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG22	11	0.16
(1,1891)	1:28:A:PHE:HA	1:68:A:VAL:HG23	11	0.16
(1,1862)	1:63:A:THR:HB	1:64:A:PRO:HD2	10	0.16
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	4	0.16
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	4	0.16
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	4	0.16
(1,1775)	1:56:A:ILE:HD11	1:48:A:LEU:HB2	8	0.16
(1,1775)	1:56:A:ILE:HD12	1:48:A:LEU:HB2	8	0.16
(1,1775)	1:56:A:ILE:HD13	1:48:A:LEU:HB2	8	0.16
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	5	0.16
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	5	0.16
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	5	0.16
(1,1754)	1:57:A:LYS:HG2	1:72:A:VAL:HB	3	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	3	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	3	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	3	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	3	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	3	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	3	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	3	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	3	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	3	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	4	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	4	0.16
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	4	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	4	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	4	0.16
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	4	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	4	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	4	0.16
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	4	0.16
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	8	0.16
(1,1443)	1:58:A:ILE:HG21	1:58:A:ILE:HA	11	0.16
(1,1443)	1:58:A:ILE:HG22	1:58:A:ILE:HA	11	0.16
(1,1443)	1:58:A:ILE:HG23	1:58:A:ILE:HA	11	0.16
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE1	1	0.16
(1,1421)	1:86:A:ARG:HD2	1:51:A:PHE:HE2	1	0.16
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	7	0.16
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	7	0.16
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	7	0.16
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	11	0.16
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	11	0.16
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB1	6	0.16
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB2	6	0.16
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB3	6	0.16
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB1	6	0.16
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB2	6	0.16
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB3	6	0.16
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB1	6	0.16
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB2	6	0.16
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB3	6	0.16
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG21	3	0.16
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG22	3	0.16
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG23	3	0.16
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD3	2	0.16
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	7	0.16
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	8	0.16
(1,1329)	1:175:A:ALA:HB1	1:178:A:LYS:HD3	12	0.16
(1,1329)	1:175:A:ALA:HB2	1:178:A:LYS:HD3	12	0.16
(1,1329)	1:175:A:ALA:HB3	1:178:A:LYS:HD3	12	0.16
(1,1270)	1:36:A:ALA:HB1	1:37:A:ILE:HD11	8	0.16
(1,1270)	1:36:A:ALA:HB1	1:37:A:ILE:HD12	8	0.16
(1,1270)	1:36:A:ALA:HB1	1:37:A:ILE:HD13	8	0.16
(1,1270)	1:36:A:ALA:HB2	1:37:A:ILE:HD11	8	0.16
(1,1270)	1:36:A:ALA:HB2	1:37:A:ILE:HD12	8	0.16
(1,1270)	1:36:A:ALA:HB2	1:37:A:ILE:HD13	8	0.16
(1,1270)	1:36:A:ALA:HB3	1:37:A:ILE:HD11	8	0.16
(1,1270)	1:36:A:ALA:HB3	1:37:A:ILE:HD12	8	0.16
(1,1270)	1:36:A:ALA:HB3	1:37:A:ILE:HD13	8	0.16
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	1	0.16
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	7	0.16
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	5	0.16
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	6	0.16
(1,1087)	1:93:A:GLU:HB3	1:93:A:GLU:HG3	11	0.16
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	5	0.16
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	8	0.16
(1,452)	1:98:A:GLY:H	1:99:A:PRO:HB2	6	0.16
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	10	0.16
(1,147)	1:22:A:GLN:H	1:21:A:GLU:HA	10	0.16
(2,70)	1:137:A:GLU:HA	1:131:A:GLN:HG2	11	0.15
(2,53)	1:58:A:ILE:HD11	1:71:A:VAL:HA	3	0.15
(2,53)	1:58:A:ILE:HD12	1:71:A:VAL:HA	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:58:A:ILE:HD13	1:71:A:VAL:HA	3	0.15
(2,14)	1:93:A:GLU:H	1:160:A:PHE:HB2	12	0.15
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	2	0.15
(1,2061)	1:140:A:VAL:HA	1:154:A:VAL:HA	1	0.15
(1,2061)	1:140:A:VAL:HA	1:154:A:VAL:HA	3	0.15
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	6	0.15
(1,2028)	1:140:A:VAL:HG21	2:4:B:G:H1'	1	0.15
(1,2028)	1:140:A:VAL:HG22	2:4:B:G:H1'	1	0.15
(1,2028)	1:140:A:VAL:HG23	2:4:B:G:H1'	1	0.15
(1,1948)	1:96:A:PHE:HD1	1:91:A:LEU:HA	11	0.15
(1,1948)	1:96:A:PHE:HD2	1:91:A:LEU:HA	11	0.15
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG21	9	0.15
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG22	9	0.15
(1,1874)	1:57:A:LYS:HD3	1:72:A:VAL:HG23	9	0.15
(1,1871)	1:177:A:VAL:HA	1:179:A:GLN:HB2	5	0.15
(1,1790)	1:103:A:VAL:HG11	1:96:A:PHE:HB2	12	0.15
(1,1790)	1:103:A:VAL:HG12	1:96:A:PHE:HB2	12	0.15
(1,1790)	1:103:A:VAL:HG13	1:96:A:PHE:HB2	12	0.15
(1,1756)	1:57:A:LYS:HE3	1:57:A:LYS:HB2	12	0.15
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG21	10	0.15
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG22	10	0.15
(1,1755)	1:57:A:LYS:HG2	1:72:A:VAL:HG23	10	0.15
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG11	3	0.15
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG12	3	0.15
(1,1739)	1:92:A:LYS:HE3	1:103:A:VAL:HG13	3	0.15
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	6	0.15
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	7	0.15
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	11	0.15
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	12	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB1	3	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB2	3	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB3	3	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB1	3	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB2	3	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB3	3	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB1	3	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB2	3	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB3	3	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB1	5	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB2	5	0.15
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB3	5	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB1	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB2	5	0.15
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB3	5	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB1	5	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB2	5	0.15
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB3	5	0.15
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	9	0.15
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	12	0.15
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG21	4	0.15
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG22	4	0.15
(1,1328)	1:118:A:ARG:HB3	1:173:A:ILE:HG23	4	0.15
(1,1167)	1:78:A:GLU:HG3	1:78:A:GLU:H	1	0.15
(1,1148)	1:34:A:VAL:HG11	1:69:A:ARG:HB3	1	0.15
(1,1148)	1:34:A:VAL:HG12	1:69:A:ARG:HB3	1	0.15
(1,1148)	1:34:A:VAL:HG13	1:69:A:ARG:HB3	1	0.15
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	5	0.15
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	5	0.15
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	5	0.15
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	6	0.15
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	6	0.15
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	6	0.15
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	1	0.15
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	1	0.15
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	1	0.15
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	8	0.15
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	8	0.15
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	8	0.15
(1,588)	1:58:A:ILE:HB	1:59:A:ALA:H	9	0.15
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	2	0.15
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	8	0.15
(1,549)	1:63:A:THR:H	1:64:A:PRO:HD2	5	0.15
(1,452)	1:98:A:GLY:H	1:99:A:PRO:HB2	2	0.15
(1,391)	1:109:A:ILE:H	1:109:A:ILE:HD11	3	0.15
(1,391)	1:109:A:ILE:H	1:109:A:ILE:HD12	3	0.15
(1,391)	1:109:A:ILE:H	1:109:A:ILE:HD13	3	0.15
(1,376)	1:57:A:LYS:H	1:57:A:LYS:HD2	8	0.15
(1,301)	1:63:A:THR:H	1:62:A:GLU:HB2	12	0.15
(2,99)	1:118:A:ARG:NH1	1:180:A:GLN:OE1	3	0.14
(2,67)	1:63:A:THR:HG21	1:65:A:ASP:HA	9	0.14
(2,67)	1:63:A:THR:HG22	1:65:A:ASP:HA	9	0.14
(2,67)	1:63:A:THR:HG23	1:65:A:ASP:HA	9	0.14
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	4	0.14
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	4	0.14
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	9	0.14
(1,2088)	1:171:A:ARG:H	1:172:A:ASP:H	1	0.14
(1,2088)	1:171:A:ARG:H	1:172:A:ASP:H	5	0.14
(1,2077)	1:176:A:GLN:HA	1:179:A:GLN:H	8	0.14
(1,2051)	1:177:A:VAL:HG21	2:2:B:C:H1'	11	0.14
(1,2051)	1:177:A:VAL:HG22	2:2:B:C:H1'	11	0.14
(1,2051)	1:177:A:VAL:HG23	2:2:B:C:H1'	11	0.14
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG11	4	0.14
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG12	4	0.14
(1,1960)	1:97:A:PHE:HD1	1:103:A:VAL:HG13	4	0.14
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG11	4	0.14
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG12	4	0.14
(1,1960)	1:97:A:PHE:HD2	1:103:A:VAL:HG13	4	0.14
(1,1948)	1:96:A:PHE:HD1	1:91:A:LEU:HA	4	0.14
(1,1948)	1:96:A:PHE:HD2	1:91:A:LEU:HA	4	0.14
(1,1945)	1:88:A:TYR:HD1	1:103:A:VAL:HB	10	0.14
(1,1945)	1:88:A:TYR:HD2	1:103:A:VAL:HB	10	0.14
(1,1862)	1:63:A:THR:HB	1:64:A:PRO:HD2	5	0.14
(1,1807)	1:48:A:LEU:HD11	1:86:A:ARG:HG2	2	0.14
(1,1807)	1:48:A:LEU:HD12	1:86:A:ARG:HG2	2	0.14
(1,1807)	1:48:A:LEU:HD13	1:86:A:ARG:HG2	2	0.14
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	1	0.14
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG21	7	0.14
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG22	7	0.14
(1,1760)	1:57:A:LYS:HE3	1:72:A:VAL:HG23	7	0.14
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG11	5	0.14
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG12	5	0.14
(1,1759)	1:57:A:LYS:HE3	1:72:A:VAL:HG13	5	0.14
(1,1640)	1:151:A:GLN:HA	1:146:A:PRO:HB3	11	0.14
(1,1621)	1:151:A:GLN:HA	1:112:A:PRO:HA	11	0.14
(1,1618)	1:151:A:GLN:HG2	1:151:A:GLN:HA	5	0.14
(1,1530)	1:21:A:GLU:HB3	1:21:A:GLU:HG3	3	0.14
(1,1528)	1:148:A:GLU:HA	1:148:A:GLU:HG3	1	0.14
(1,1398)	1:22:A:GLN:HB3	1:23:A:GLU:H	11	0.14
(1,1397)	1:22:A:GLN:HB2	1:23:A:GLU:H	3	0.14
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	3	0.14
(1,1276)	1:92:A:LYS:HD3	1:92:A:LYS:HA	7	0.14
(1,1167)	1:78:A:GLU:HG3	1:78:A:GLU:H	12	0.14
(1,1127)	1:128:A:ASN:HB3	1:129:A:GLU:H	6	0.14
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	3	0.14
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	7	0.14
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	7	0.14
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	7	0.14
(1,940)	1:169:A:LYS:HA	1:172:A:ASP:HB2	9	0.14
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	5	0.14
(1,552)	1:139:A:VAL:H	1:156:A:ILE:HG12	9	0.14
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD11	12	0.14
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD12	12	0.14
(1,538)	1:45:A:ILE:H	1:37:A:ILE:HD13	12	0.14
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	3	0.14
(1,441)	1:29:A:ILE:H	1:68:A:VAL:HA	5	0.14
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	1	0.14
(1,354)	1:58:A:ILE:H	1:57:A:LYS:HA	11	0.14
(1,301)	1:63:A:THR:H	1:62:A:GLU:HB2	10	0.14
(1,144)	1:92:A:LYS:H	1:92:A:LYS:HG3	11	0.14
(1,134)	1:101:A:GLU:H	1:101:A:GLU:HB3	11	0.14
(1,51)	1:62:A:GLU:H	1:62:A:GLU:HB3	6	0.14
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	3	0.13
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	12	0.13
(1,2097)	1:180:A:GLN:H	1:181:A:HIS:H	7	0.13
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	12	0.13
(1,2054)	1:139:A:VAL:HA	2:5:B:A:H2	10	0.13
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	4	0.13
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	7	0.13
(1,1986)	1:88:A:TYR:HE1	1:103:A:VAL:HB	6	0.13
(1,1986)	1:88:A:TYR:HE2	1:103:A:VAL:HB	6	0.13
(1,1940)	1:28:A:PHE:HD1	1:106:A:GLU:HB2	3	0.13
(1,1940)	1:28:A:PHE:HD2	1:106:A:GLU:HB2	3	0.13
(1,1912)	1:156:A:ILE:HG21	1:166:A:ALA:HA	6	0.13
(1,1912)	1:156:A:ILE:HG22	1:166:A:ALA:HA	6	0.13
(1,1912)	1:156:A:ILE:HG23	1:166:A:ALA:HA	6	0.13
(1,1898)	1:77:A:PRO:HD3	1:78:A:GLU:HG3	8	0.13
(1,1890)	1:28:A:PHE:HA	1:68:A:VAL:HB	5	0.13
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG11	12	0.13
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG12	12	0.13
(1,1870)	1:118:A:ARG:HD2	1:177:A:VAL:HG13	12	0.13
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	2	0.13
(1,1666)	1:145:A:THR:HG21	1:144:A:GLN:HA	1	0.13
(1,1666)	1:145:A:THR:HG22	1:144:A:GLN:HA	1	0.13
(1,1666)	1:145:A:THR:HG23	1:144:A:GLN:HA	1	0.13
(1,1666)	1:145:A:THR:HG21	1:144:A:GLN:HA	6	0.13
(1,1666)	1:145:A:THR:HG22	1:144:A:GLN:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:145:A:THR:HG23	1:144:A:GLN:HA	6	0.13
(1,1654)	1:105:A:LEU:HD21	1:91:A:LEU:HG	12	0.13
(1,1654)	1:105:A:LEU:HD22	1:91:A:LEU:HG	12	0.13
(1,1654)	1:105:A:LEU:HD23	1:91:A:LEU:HG	12	0.13
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	2	0.13
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	2	0.13
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	2	0.13
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	2	0.13
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	2	0.13
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	2	0.13
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	2	0.13
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	2	0.13
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	2	0.13
(1,1445)	1:146:A:PRO:HD3	1:145:A:THR:HA	6	0.13
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB1	6	0.13
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB2	6	0.13
(1,1377)	1:146:A:PRO:HG3	1:113:A:ALA:HB3	6	0.13
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD11	12	0.13
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD12	12	0.13
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD13	12	0.13
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB1	4	0.13
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB2	4	0.13
(1,1363)	1:29:A:ILE:HD11	1:33:A:ALA:HB3	4	0.13
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB1	4	0.13
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB2	4	0.13
(1,1363)	1:29:A:ILE:HD12	1:33:A:ALA:HB3	4	0.13
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB1	4	0.13
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB2	4	0.13
(1,1363)	1:29:A:ILE:HD13	1:33:A:ALA:HB3	4	0.13
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	1	0.13
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	1	0.13
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	1	0.13
(1,1220)	1:146:A:PRO:HD2	1:144:A:GLN:HG2	1	0.13
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	4	0.13
(1,1125)	1:128:A:ASN:HB2	1:125:A:LYS:HA	5	0.13
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	2	0.13
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	2	0.13
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG3	7	0.13
(1,1047)	1:34:A:VAL:HG11	1:31:A:ALA:HA	12	0.13
(1,1047)	1:34:A:VAL:HG12	1:31:A:ALA:HA	12	0.13
(1,1047)	1:34:A:VAL:HG13	1:31:A:ALA:HA	12	0.13
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	10	0.13
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	10	0.13
(1,963)	1:105:A:LEU:HD21	1:106:A:GLU:HB3	8	0.13
(1,963)	1:105:A:LEU:HD22	1:106:A:GLU:HB3	8	0.13
(1,963)	1:105:A:LEU:HD23	1:106:A:GLU:HB3	8	0.13
(1,940)	1:169:A:LYS:HA	1:172:A:ASP:HB2	8	0.13
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	2	0.13
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	3	0.13
(1,775)	1:150:A:GLU:HG3	1:150:A:GLU:HB2	10	0.13
(1,723)	1:111:A:VAL:HB	1:112:A:PRO:HD2	1	0.13
(1,602)	1:150:A:GLU:HG2	1:150:A:GLU:H	2	0.13
(1,559)	1:83:A:ALA:H	1:79:A:ALA:HA	7	0.13
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	5	0.13
(1,478)	1:93:A:GLU:H	1:94:A:GLU:HB3	7	0.13
(1,333)	1:32:A:GLN:H	1:32:A:GLN:HB3	9	0.13
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	2	0.13
(1,221)	1:91:A:LEU:H	1:91:A:LEU:HG	9	0.13
(2,73)	1:22:A:GLN:HA	1:20:A:PRO:HB3	10	0.12
(2,53)	1:58:A:ILE:HD11	1:71:A:VAL:HA	5	0.12
(2,53)	1:58:A:ILE:HD12	1:71:A:VAL:HA	5	0.12
(2,53)	1:58:A:ILE:HD13	1:71:A:VAL:HA	5	0.12
(2,23)	1:154:A:VAL:H	1:155:A:LYS:HE2	7	0.12
(2,18)	1:174:A:LEU:H	1:170:A:ILE:HB	2	0.12
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	8	0.12
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	8	0.12
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	8	0.12
(1,2093)	1:176:A:GLN:H	1:177:A:VAL:H	1	0.12
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	5	0.12
(1,2064)	1:28:A:PHE:HA	1:70:A:MET:HA	12	0.12
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	3	0.12
(1,2027)	1:118:A:ARG:HB2	2:2:B:C:H1'	11	0.12
(1,2027)	1:118:A:ARG:HB3	2:2:B:C:H1'	11	0.12
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD11	10	0.12
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD12	10	0.12
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD13	10	0.12
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	6	0.12
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	6	0.12
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	6	0.12
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	11	0.12
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	11	0.12
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	11	0.12
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD22	1	0.12
(1,1599)	1:115:A:ALA:HB1	1:174:A:LEU:HD23	1	0.12
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD21	1	0.12
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD22	1	0.12
(1,1599)	1:115:A:ALA:HB2	1:174:A:LEU:HD23	1	0.12
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD21	1	0.12
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD22	1	0.12
(1,1599)	1:115:A:ALA:HB3	1:174:A:LEU:HD23	1	0.12
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG11	5	0.12
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG12	5	0.12
(1,1598)	1:107:A:THR:HG21	1:25:A:VAL:HG13	5	0.12
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG11	5	0.12
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG12	5	0.12
(1,1598)	1:107:A:THR:HG22	1:25:A:VAL:HG13	5	0.12
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG11	5	0.12
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG12	5	0.12
(1,1598)	1:107:A:THR:HG23	1:25:A:VAL:HG13	5	0.12
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	2	0.12
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	2	0.12
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	2	0.12
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	6	0.12
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	6	0.12
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	6	0.12
(1,1500)	1:54:A:ALA:HB1	1:55:A:SER:HB2	7	0.12
(1,1500)	1:54:A:ALA:HB2	1:55:A:SER:HB2	7	0.12
(1,1500)	1:54:A:ALA:HB3	1:55:A:SER:HB2	7	0.12
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD11	6	0.12
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD12	6	0.12
(1,1370)	1:48:A:LEU:HG	1:56:A:ILE:HD13	6	0.12
(1,1351)	1:34:A:VAL:HG11	1:58:A:ILE:HB	3	0.12
(1,1351)	1:34:A:VAL:HG12	1:58:A:ILE:HB	3	0.12
(1,1351)	1:34:A:VAL:HG13	1:58:A:ILE:HB	3	0.12
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	3	0.12
(1,1330)	1:178:A:LYS:HG2	1:178:A:LYS:HD2	10	0.12
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD1	7	0.12
(1,1310)	1:91:A:LEU:HD21	1:88:A:TYR:HD2	7	0.12
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD1	7	0.12
(1,1310)	1:91:A:LEU:HD22	1:88:A:TYR:HD2	7	0.12
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD1	7	0.12
(1,1310)	1:91:A:LEU:HD23	1:88:A:TYR:HD2	7	0.12
(1,1280)	1:93:A:GLU:HG2	1:90:A:LYS:HA	1	0.12
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	5	0.12
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	10	0.12
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	11	0.12
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	12	0.12
(1,1065)	1:166:A:ALA:HA	1:130:A:LEU:HD21	4	0.12
(1,1065)	1:166:A:ALA:HA	1:130:A:LEU:HD22	4	0.12
(1,1065)	1:166:A:ALA:HA	1:130:A:LEU:HD23	4	0.12
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG21	7	0.12
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG22	7	0.12
(1,1063)	1:27:A:VAL:HB	1:71:A:VAL:HG23	7	0.12
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	2	0.12
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	9	0.12
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	12	0.12
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	5	0.12
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	5	0.12
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	5	0.12
(1,992)	1:74:A:THR:HG21	1:75:A:GLY:HA3	11	0.12
(1,992)	1:74:A:THR:HG22	1:75:A:GLY:HA3	11	0.12
(1,992)	1:74:A:THR:HG23	1:75:A:GLY:HA3	11	0.12
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	4	0.12
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	4	0.12
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	4	0.12
(1,910)	1:56:A:ILE:HB	1:56:A:ILE:HD11	1	0.12
(1,910)	1:56:A:ILE:HB	1:56:A:ILE:HD12	1	0.12
(1,910)	1:56:A:ILE:HB	1:56:A:ILE:HD13	1	0.12
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	1	0.12
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	5	0.12
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	8	0.12
(1,827)	1:48:A:LEU:HG	1:48:A:LEU:HB2	9	0.12
(1,777)	1:62:A:GLU:HA	1:62:A:GLU:HG2	10	0.12
(1,692)	1:133:A:LEU:HD21	1:133:A:LEU:HA	7	0.12
(1,692)	1:133:A:LEU:HD22	1:133:A:LEU:HA	7	0.12
(1,692)	1:133:A:LEU:HD23	1:133:A:LEU:HA	7	0.12
(1,565)	1:151:A:GLN:H	1:147:A:ASP:H	5	0.12
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	12	0.12
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD11	9	0.12
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD12	9	0.12
(1,493)	1:36:A:ALA:H	1:37:A:ILE:HD13	9	0.12
(1,453)	1:65:A:ASP:H	1:64:A:PRO:HB2	8	0.12
(1,333)	1:32:A:GLN:H	1:32:A:GLN:HB3	10	0.12
(1,333)	1:32:A:GLN:H	1:32:A:GLN:HB3	11	0.12
(1,218)	1:96:A:PHE:H	1:94:A:GLU:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:74:A:THR:H	1:24:A:THR:HG21	5	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG22	5	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG23	5	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG21	8	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG22	8	0.12
(1,29)	1:74:A:THR:H	1:24:A:THR:HG23	8	0.12
(2,98)	1:118:A:ARG:NH2	1:180:A:GLN:OE1	3	0.11
(2,53)	1:58:A:ILE:HD11	1:71:A:VAL:HA	1	0.11
(2,53)	1:58:A:ILE:HD12	1:71:A:VAL:HA	1	0.11
(2,53)	1:58:A:ILE:HD13	1:71:A:VAL:HA	1	0.11
(2,19)	1:165:A:MET:H	1:156:A:ILE:HD11	4	0.11
(2,19)	1:165:A:MET:H	1:156:A:ILE:HD12	4	0.11
(2,19)	1:165:A:MET:H	1:156:A:ILE:HD13	4	0.11
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG11	1	0.11
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG12	1	0.11
(2,9)	1:117:A:GLY:H	1:154:A:VAL:HG13	1	0.11
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	2	0.11
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	6	0.11
(1,2094)	1:177:A:VAL:H	1:178:A:LYS:H	8	0.11
(1,2085)	1:168:A:ARG:H	1:169:A:LYS:H	8	0.11
(1,2082)	1:165:A:MET:H	1:166:A:ALA:H	11	0.11
(1,2070)	1:169:A:LYS:HA	1:172:A:ASP:H	8	0.11
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	3	0.11
(1,2062)	1:71:A:VAL:HA	1:58:A:ILE:HA	4	0.11
(1,2058)	1:107:A:THR:HA	1:27:A:VAL:HA	12	0.11
(1,2044)	2:4:B:G:H4'	2:5:B:A:H8	4	0.11
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	11	0.11
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD11	9	0.11
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD12	9	0.11
(1,1978)	1:97:A:PHE:HE1	1:91:A:LEU:HD13	9	0.11
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD11	9	0.11
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD12	9	0.11
(1,1978)	1:97:A:PHE:HE2	1:91:A:LEU:HD13	9	0.11
(1,1756)	1:57:A:LYS:HE2	1:57:A:LYS:HB2	6	0.11
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	1	0.11
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	11	0.11
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	5	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	5	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	5	0.11
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	7	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	7	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	8	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	8	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	8	0.11
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	9	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	9	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	9	0.11
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	10	0.11
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	10	0.11
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	10	0.11
(1,1628)	1:170:A:ILE:HA	1:170:A:ILE:HG21	2	0.11
(1,1628)	1:170:A:ILE:HA	1:170:A:ILE:HG22	2	0.11
(1,1628)	1:170:A:ILE:HA	1:170:A:ILE:HG23	2	0.11
(1,1608)	1:34:A:VAL:HG11	1:29:A:ILE:HD11	2	0.11
(1,1608)	1:34:A:VAL:HG11	1:29:A:ILE:HD12	2	0.11
(1,1608)	1:34:A:VAL:HG11	1:29:A:ILE:HD13	2	0.11
(1,1608)	1:34:A:VAL:HG12	1:29:A:ILE:HD11	2	0.11
(1,1608)	1:34:A:VAL:HG12	1:29:A:ILE:HD12	2	0.11
(1,1608)	1:34:A:VAL:HG12	1:29:A:ILE:HD13	2	0.11
(1,1608)	1:34:A:VAL:HG13	1:29:A:ILE:HD11	2	0.11
(1,1608)	1:34:A:VAL:HG13	1:29:A:ILE:HD12	2	0.11
(1,1608)	1:34:A:VAL:HG13	1:29:A:ILE:HD13	2	0.11
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	3	0.11
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	3	0.11
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	3	0.11
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	5	0.11
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	5	0.11
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	5	0.11
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	7	0.11
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	7	0.11
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	7	0.11
(1,1466)	1:131:A:GLN:HG3	1:131:A:GLN:HA	10	0.11
(1,1446)	1:145:A:THR:HG21	1:145:A:THR:HA	5	0.11
(1,1446)	1:145:A:THR:HG22	1:145:A:THR:HA	5	0.11
(1,1446)	1:145:A:THR:HG23	1:145:A:THR:HA	5	0.11
(1,1446)	1:145:A:THR:HG21	1:145:A:THR:HA	7	0.11
(1,1446)	1:145:A:THR:HG22	1:145:A:THR:HA	7	0.11
(1,1446)	1:145:A:THR:HG23	1:145:A:THR:HA	7	0.11
(1,1412)	1:171:A:ARG:HB3	1:168:A:ARG:HA	4	0.11
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD1	10	0.11
(1,1348)	1:93:A:GLU:HG3	1:96:A:PHE:HD2	10	0.11
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	5	0.11
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG22	5	0.11
(1,1333)	1:118:A:ARG:HD3	1:173:A:ILE:HG23	5	0.11
(1,1326)	1:118:A:ARG:HB3	1:118:A:ARG:HG2	2	0.11
(1,1326)	1:118:A:ARG:HB2	1:118:A:ARG:HG2	5	0.11
(1,1326)	1:118:A:ARG:HB2	1:118:A:ARG:HG3	6	0.11
(1,1264)	1:174:A:LEU:HD21	1:179:A:GLN:HG3	1	0.11
(1,1264)	1:174:A:LEU:HD22	1:179:A:GLN:HG3	1	0.11
(1,1264)	1:174:A:LEU:HD23	1:179:A:GLN:HG3	1	0.11
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	9	0.11
(1,1128)	1:37:A:ILE:HD11	1:90:A:LYS:HD2	9	0.11
(1,1128)	1:37:A:ILE:HD12	1:90:A:LYS:HD2	9	0.11
(1,1128)	1:37:A:ILE:HD13	1:90:A:LYS:HD2	9	0.11
(1,1123)	1:86:A:ARG:HD3	1:86:A:ARG:HG2	6	0.11
(1,1118)	1:91:A:LEU:HD21	1:30:A:PRO:HD3	11	0.11
(1,1118)	1:91:A:LEU:HD22	1:30:A:PRO:HD3	11	0.11
(1,1118)	1:91:A:LEU:HD23	1:30:A:PRO:HD3	11	0.11
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	3	0.11
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	4	0.11
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	6	0.11
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	8	0.11
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	10	0.11
(1,962)	1:148:A:GLU:HG2	1:148:A:GLU:HB3	2	0.11
(1,960)	1:153:A:ILE:HG21	1:154:A:VAL:HB	10	0.11
(1,960)	1:153:A:ILE:HG22	1:154:A:VAL:HB	10	0.11
(1,960)	1:153:A:ILE:HG23	1:154:A:VAL:HB	10	0.11
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD11	4	0.11
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD12	4	0.11
(1,879)	1:87:A:ILE:HA	1:48:A:LEU:HD13	4	0.11
(1,558)	1:83:A:ALA:H	1:86:A:ARG:HB2	12	0.11
(1,521)	1:119:A:VAL:H	1:117:A:GLY:HA3	12	0.11
(1,501)	1:118:A:ARG:H	1:118:A:ARG:HG3	8	0.11
(1,453)	1:65:A:ASP:H	1:64:A:PRO:HB2	11	0.11
(1,452)	1:98:A:GLY:H	1:99:A:PRO:HB2	3	0.11
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	9	0.11
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG11	2	0.11
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG12	2	0.11
(1,394)	1:26:A:HIS:H	1:25:A:VAL:HG13	2	0.11
(1,274)	1:53:A:SER:H	1:53:A:SER:HB3	2	0.11
(1,274)	1:53:A:SER:H	1:53:A:SER:HB3	4	0.11
(1,225)	1:91:A:LEU:H	1:91:A:LEU:HD11	3	0.11
(1,225)	1:91:A:LEU:H	1:91:A:LEU:HD12	3	0.11
(1,225)	1:91:A:LEU:H	1:91:A:LEU:HD13	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:149:A:ASN:H	1:149:A:ASN:HB2	3	0.11
(2,37)	1:105:A:LEU:HD11	1:29:A:ILE:HG12	7	0.1
(2,37)	1:105:A:LEU:HD12	1:29:A:ILE:HG12	7	0.1
(2,37)	1:105:A:LEU:HD13	1:29:A:ILE:HG12	7	0.1
(1,2098)	1:181:A:HIS:H	1:182:A:GLN:H	5	0.1
(1,2097)	1:180:A:GLN:H	1:181:A:HIS:H	2	0.1
(1,2094)	1:177:A:VAL:H	1:178:A:LYS:H	5	0.1
(1,2094)	1:177:A:VAL:H	1:178:A:LYS:H	9	0.1
(1,2094)	1:177:A:VAL:H	1:178:A:LYS:H	11	0.1
(1,2088)	1:171:A:ARG:H	1:172:A:ASP:H	4	0.1
(1,2085)	1:168:A:ARG:H	1:169:A:LYS:H	2	0.1
(1,2082)	1:165:A:MET:H	1:166:A:ALA:H	8	0.1
(1,2046)	1:120:A:ILE:HG21	2:5:B:A:H1'	10	0.1
(1,2046)	1:120:A:ILE:HG22	2:5:B:A:H1'	10	0.1
(1,2046)	1:120:A:ILE:HG23	2:5:B:A:H1'	10	0.1
(1,2038)	2:4:B:G:H3'	2:4:B:G:H8	8	0.1
(1,2029)	2:6:B:C:H2'	2:7:B:U:H1'	1	0.1
(1,2023)	1:118:A:ARG:HD3	2:2:B:C:H2'	8	0.1
(1,1908)	1:18:A:MET:HA	1:19:A:PRO:HD2	4	0.1
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD11	6	0.1
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD12	6	0.1
(1,1905)	1:110:A:ARG:HD3	1:153:A:ILE:HD13	6	0.1
(1,1851)	1:153:A:ILE:HG21	1:141:A:PRO:HD3	3	0.1
(1,1851)	1:153:A:ILE:HG22	1:141:A:PRO:HD3	3	0.1
(1,1851)	1:153:A:ILE:HG23	1:141:A:PRO:HD3	3	0.1
(1,1810)	1:174:A:LEU:HD21	1:178:A:LYS:HD2	5	0.1
(1,1810)	1:174:A:LEU:HD22	1:178:A:LYS:HD2	5	0.1
(1,1810)	1:174:A:LEU:HD23	1:178:A:LYS:HD2	5	0.1
(1,1801)	1:107:A:THR:HG21	1:25:A:VAL:HA	12	0.1
(1,1801)	1:107:A:THR:HG22	1:25:A:VAL:HA	12	0.1
(1,1801)	1:107:A:THR:HG23	1:25:A:VAL:HA	12	0.1
(1,1800)	1:133:A:LEU:HD11	1:133:A:LEU:HB2	7	0.1
(1,1800)	1:133:A:LEU:HD12	1:133:A:LEU:HB2	7	0.1
(1,1800)	1:133:A:LEU:HD13	1:133:A:LEU:HB2	7	0.1
(1,1800)	1:133:A:LEU:HD11	1:133:A:LEU:HB2	11	0.1
(1,1800)	1:133:A:LEU:HD12	1:133:A:LEU:HB2	11	0.1
(1,1800)	1:133:A:LEU:HD13	1:133:A:LEU:HB2	11	0.1
(1,1796)	1:114:A:SER:HA	1:112:A:PRO:HG2	4	0.1
(1,1722)	1:76:A:PRO:HB2	1:77:A:PRO:HG2	3	0.1
(1,1675)	1:136:A:ALA:HB1	1:166:A:ALA:HA	12	0.1
(1,1675)	1:136:A:ALA:HB2	1:166:A:ALA:HA	12	0.1
(1,1675)	1:136:A:ALA:HB3	1:166:A:ALA:HA	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:105:A:LEU:HG	1:30:A:PRO:HD3	10	0.1
(1,1638)	1:25:A:VAL:HG21	1:25:A:VAL:HA	1	0.1
(1,1638)	1:25:A:VAL:HG22	1:25:A:VAL:HA	1	0.1
(1,1638)	1:25:A:VAL:HG23	1:25:A:VAL:HA	1	0.1
(1,1587)	1:104:A:LYS:HE2	1:104:A:LYS:HG2	3	0.1
(1,1556)	1:174:A:LEU:HD21	1:174:A:LEU:HB2	12	0.1
(1,1556)	1:174:A:LEU:HD22	1:174:A:LEU:HB2	12	0.1
(1,1556)	1:174:A:LEU:HD23	1:174:A:LEU:HB2	12	0.1
(1,1537)	1:101:A:GLU:HA	1:101:A:GLU:HB2	2	0.1
(1,1520)	1:179:A:GLN:HA	1:179:A:GLN:HG3	10	0.1
(1,1438)	1:105:A:LEU:HD21	1:105:A:LEU:HA	12	0.1
(1,1438)	1:105:A:LEU:HD22	1:105:A:LEU:HA	12	0.1
(1,1438)	1:105:A:LEU:HD23	1:105:A:LEU:HA	12	0.1
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	2	0.1
(1,1335)	1:87:A:ILE:HA	1:87:A:ILE:HG12	6	0.1
(1,1326)	1:118:A:ARG:HB2	1:118:A:ARG:HG2	3	0.1
(1,1311)	1:91:A:LEU:HD21	1:90:A:LYS:HG3	1	0.1
(1,1311)	1:91:A:LEU:HD22	1:90:A:LYS:HG3	1	0.1
(1,1311)	1:91:A:LEU:HD23	1:90:A:LYS:HG3	1	0.1
(1,1215)	1:148:A:GLU:HG3	1:148:A:GLU:HB2	12	0.1
(1,1112)	1:92:A:LYS:HD3	1:92:A:LYS:HG2	9	0.1
(1,1078)	1:48:A:LEU:HD21	1:48:A:LEU:HA	4	0.1
(1,1078)	1:48:A:LEU:HD22	1:48:A:LEU:HA	4	0.1
(1,1078)	1:48:A:LEU:HD23	1:48:A:LEU:HA	4	0.1
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	1	0.1
(1,1021)	1:141:A:PRO:HG3	1:141:A:PRO:HB3	5	0.1
(1,592)	1:58:A:ILE:HG21	1:58:A:ILE:H	11	0.1
(1,592)	1:58:A:ILE:HG22	1:58:A:ILE:H	11	0.1
(1,592)	1:58:A:ILE:HG23	1:58:A:ILE:H	11	0.1
(1,435)	1:147:A:ASP:H	1:146:A:PRO:HD3	12	0.1
(1,365)	1:102:A:GLU:H	1:102:A:GLU:HB3	3	0.1
(1,261)	1:94:A:GLU:H	1:94:A:GLU:HG3	3	0.1
(1,221)	1:91:A:LEU:H	1:91:A:LEU:HG	3	0.1
(1,40)	1:57:A:LYS:H	1:73:A:ILE:HD11	11	0.1
(1,40)	1:57:A:LYS:H	1:73:A:ILE:HD12	11	0.1
(1,40)	1:57:A:LYS:H	1:73:A:ILE:HD13	11	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found