



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 6UJV / pdb_00006ujv
BMRB ID : 30503
Title : Model of the HIV-1 gp41 membrane-proximal external region, transmembrane domain and cytoplasmic tail (LLP2)
Authors : Piai, A.; Fu, Q.; Cai, Y.; Ghantous, F.; Xiao, T.; Shaik, M.M.; Peng, H.; Rits-Volloch, S.; Liu, Z.; Chen, W.; Seaman, M.S.; Chen, B.; Chou, J.J.
Deposited on : 2019-10-03

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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

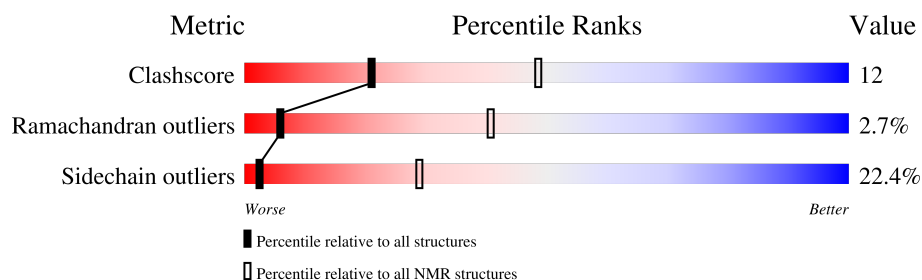
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 9%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	129	
1	B	129	
1	C	129	

2 Ensemble composition and analysis

This entry contains 15 models. Model 9 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:660-A:716, A:739-A:785, B:660-B:716, B:739-B:788, C:660-C:716, C:739-C:783 (313)	1.04	9

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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5577 atoms, of which 2859 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein GP41.

Mol	Chain	Residues	Atoms					Trace
1	A	107	Total	C	H	N	O	0
			1859	595	953	163	148	
1	B	107	Total	C	H	N	O	0
			1859	595	953	163	148	
1	C	107	Total	C	H	N	O	0
			1859	595	953	163	148	

There are 21 discrepancies between the modelled and reference sequences:

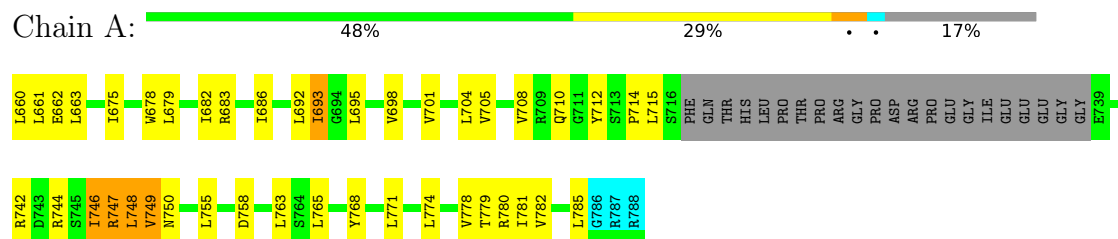
Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ARG	LYS	conflict	UNP A0A060KRW4
A	684	ILE	LEU	conflict	UNP A0A060KRW4
A	687	ILE	MET	conflict	UNP A0A060KRW4
A	691	SER	GLY	conflict	UNP A0A060KRW4
A	704	LEU	ILE	conflict	UNP A0A060KRW4
A	723	THR	ILE	conflict	UNP A0A060KRW4
A	764	SER	CYS	engineered mutation	UNP A0A060KRW4
B	683	ARG	LYS	conflict	UNP A0A060KRW4
B	684	ILE	LEU	conflict	UNP A0A060KRW4
B	687	ILE	MET	conflict	UNP A0A060KRW4
B	691	SER	GLY	conflict	UNP A0A060KRW4
B	704	LEU	ILE	conflict	UNP A0A060KRW4
B	723	THR	ILE	conflict	UNP A0A060KRW4
B	764	SER	CYS	engineered mutation	UNP A0A060KRW4
C	683	ARG	LYS	conflict	UNP A0A060KRW4
C	684	ILE	LEU	conflict	UNP A0A060KRW4
C	687	ILE	MET	conflict	UNP A0A060KRW4
C	691	SER	GLY	conflict	UNP A0A060KRW4
C	704	LEU	ILE	conflict	UNP A0A060KRW4
C	723	THR	ILE	conflict	UNP A0A060KRW4
C	764	SER	CYS	engineered mutation	UNP A0A060KRW4

4 Residue-property plots [i](#)

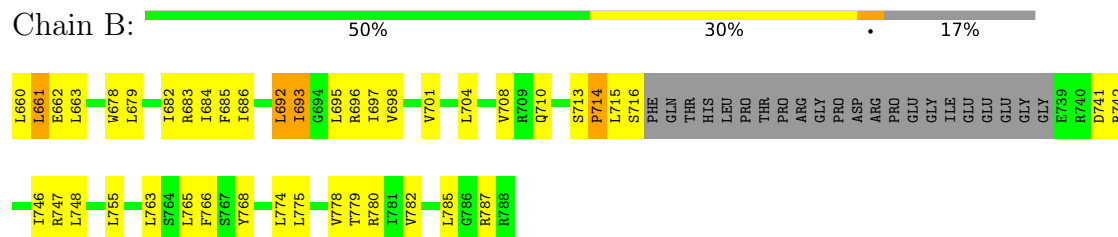
4.1 Average score per residue in the NMR ensemble

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.

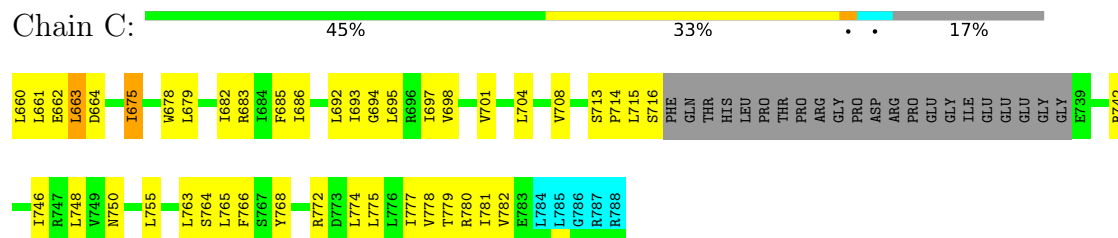
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

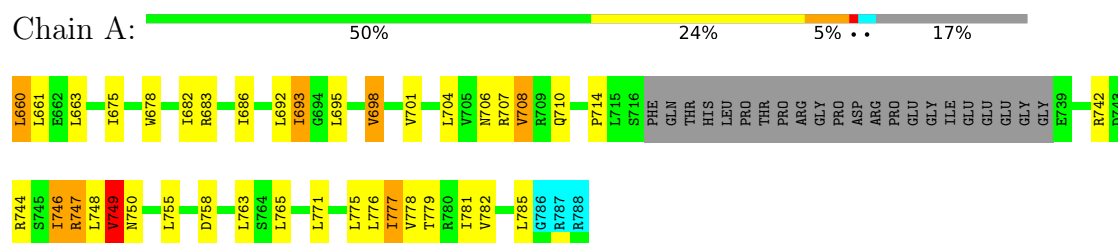


4.2 Scores per residue for each member of the ensemble

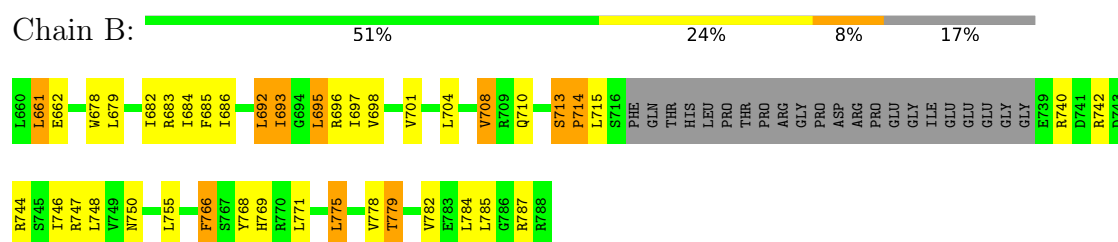
Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

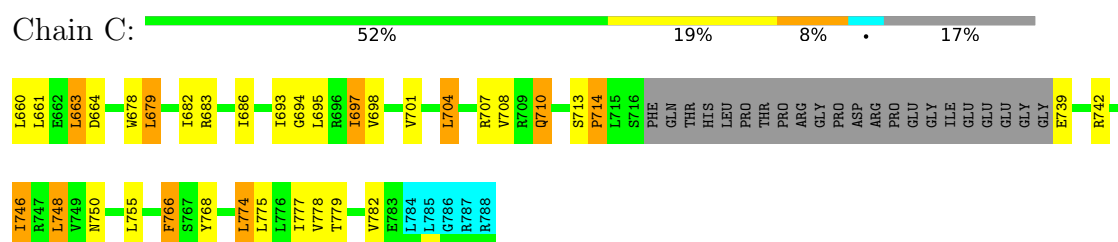
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

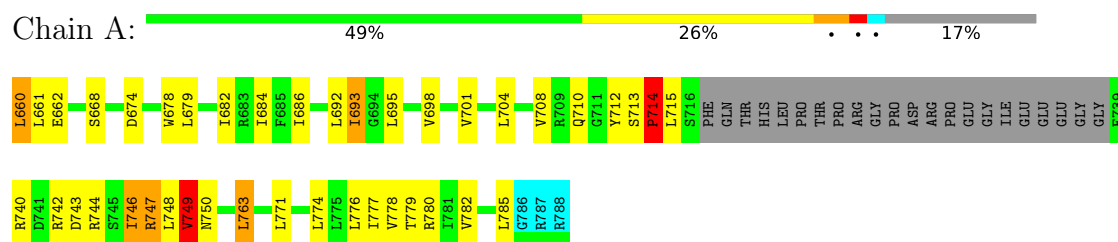


• Molecule 1: Envelope glycoprotein GP41



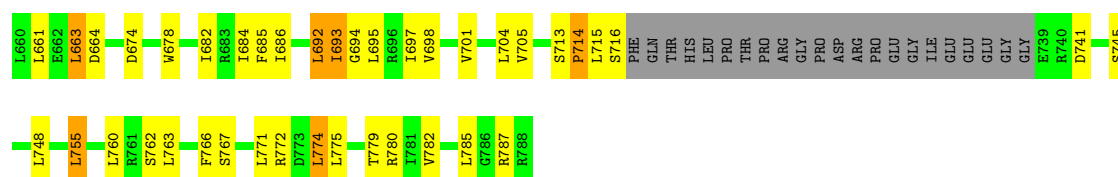
4.2.2 Score per residue for model 2

• Molecule 1: Envelope glycoprotein GP41



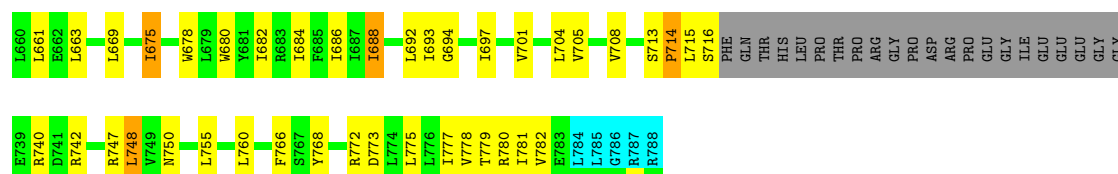
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

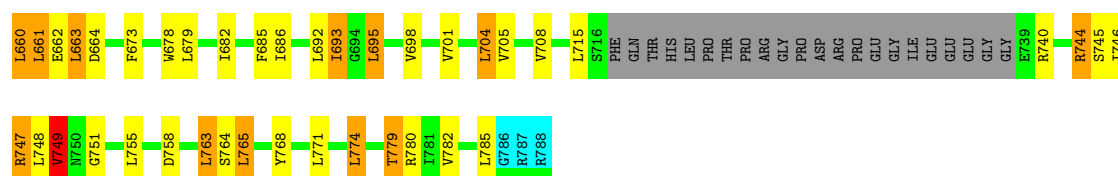
Chain C: 48% 28% 17%



4.2.3 Score per residue for model 3

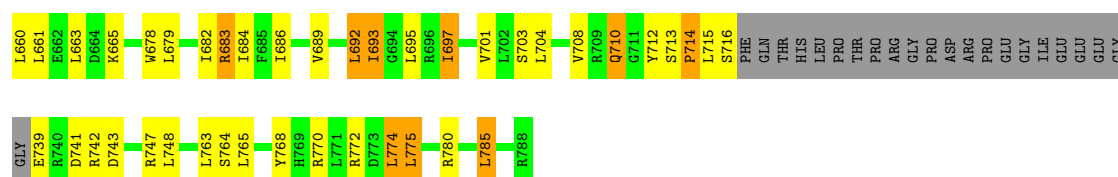
• Molecule 1: Envelope glycoprotein GP41

Chain A: 50% 21% 9% 17%



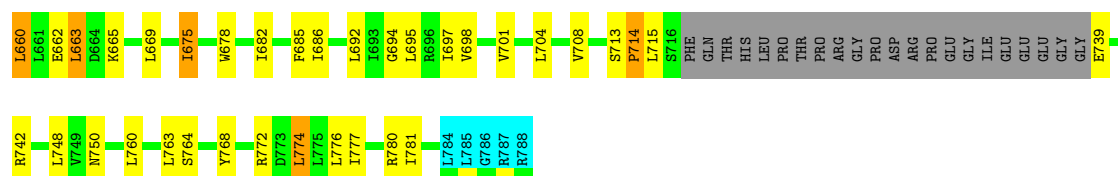
• Molecule 1: Envelope glycoprotein GP41

Chain B: 51% 25% 7% 17%



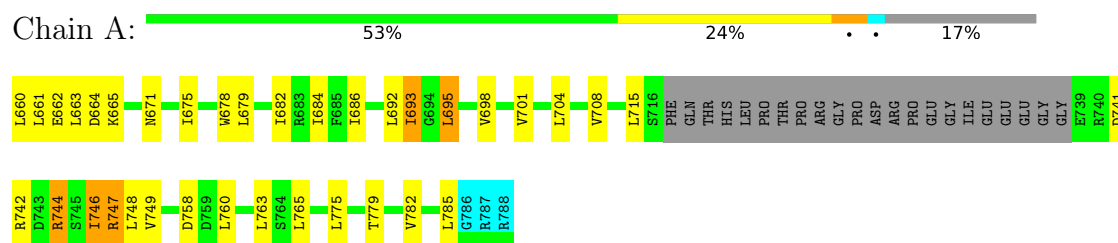
• Molecule 1: Envelope glycoprotein GP41

Chain C: 52% 23% 17%

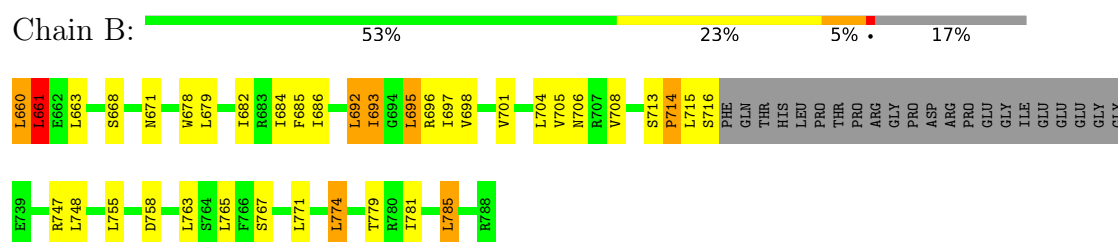


4.2.4 Score per residue for model 4

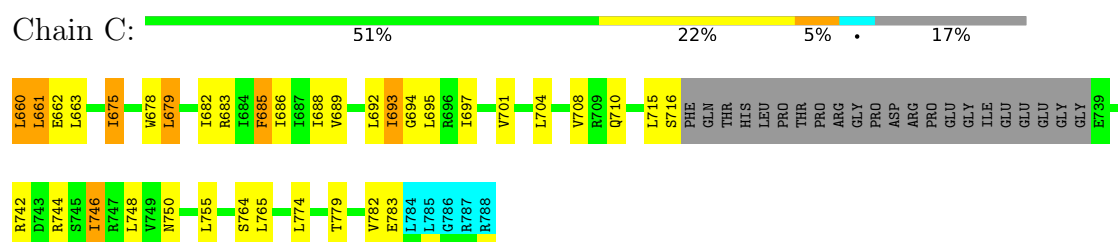
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

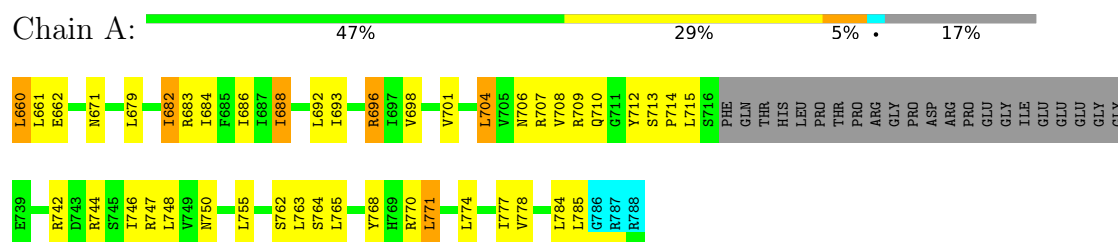


• Molecule 1: Envelope glycoprotein GP41



4.2.5 Score per residue for model 5

• Molecule 1: Envelope glycoprotein GP41

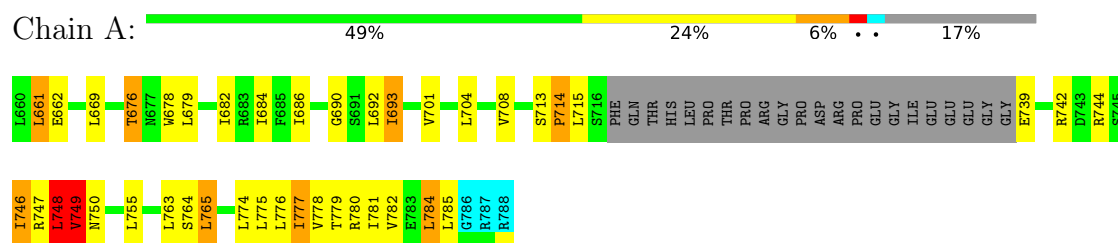


• Molecule 1: Envelope glycoprotein GP41

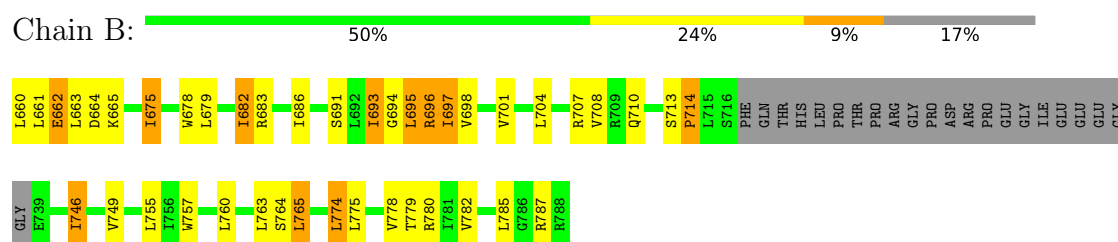


4.2.7 Score per residue for model 7

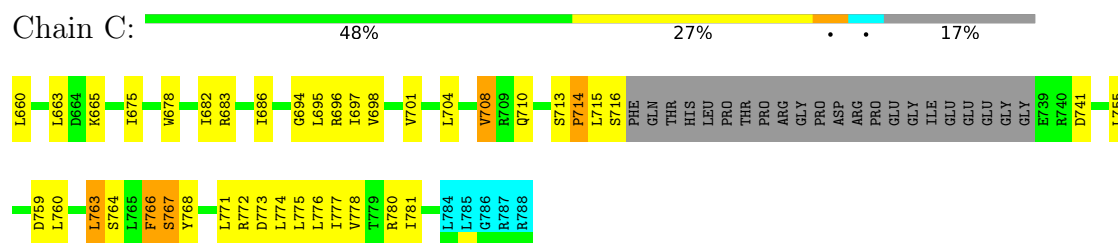
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

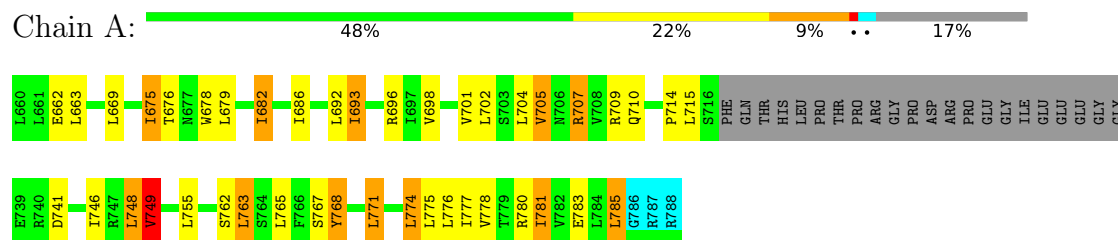


- Molecule 1: Envelope glycoprotein GP41



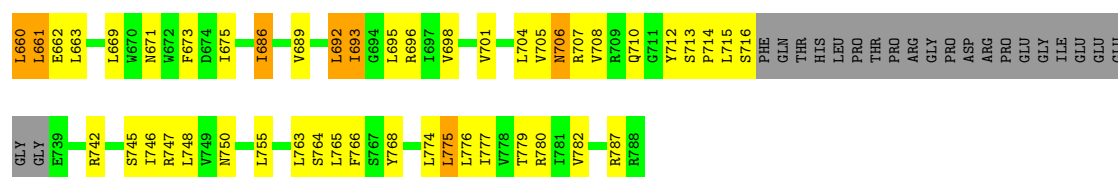
4.2.8 Score per residue for model 8

- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41



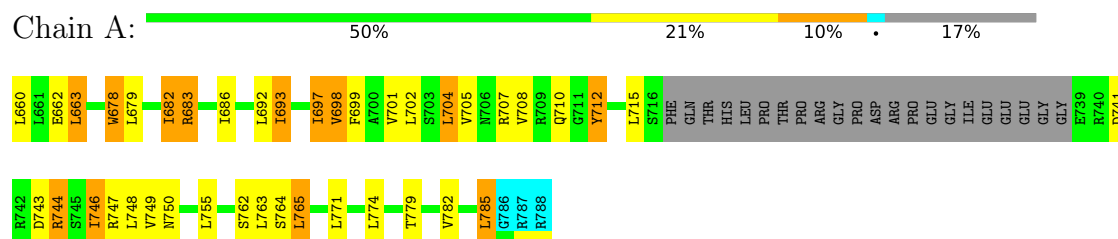


• Molecule 1: Envelope glycoprotein GP41

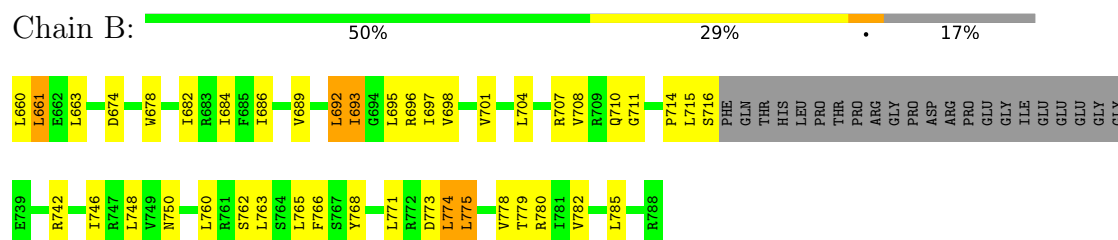


4.2.9 Score per residue for model 9 (medoid)

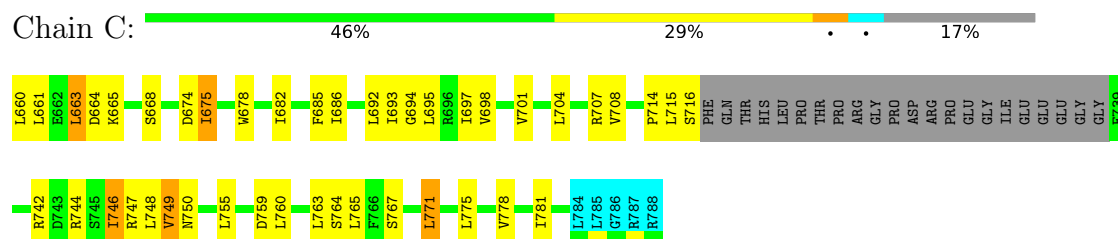
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

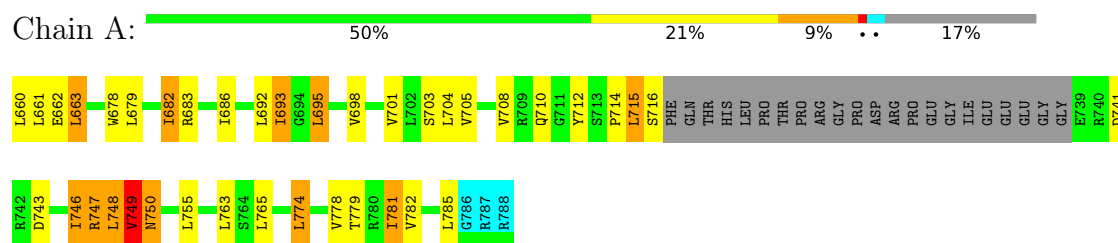


• Molecule 1: Envelope glycoprotein GP41



4.2.10 Score per residue for model 10

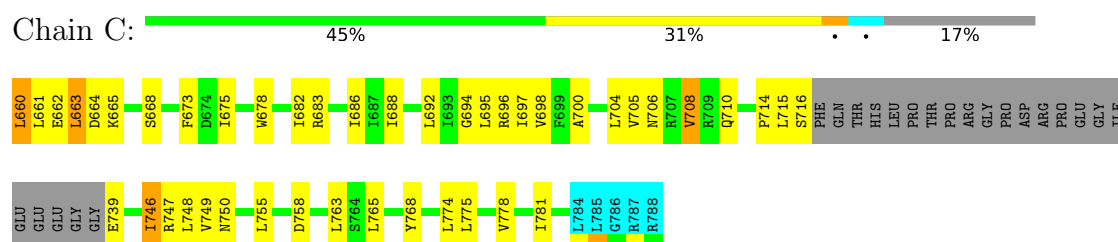
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

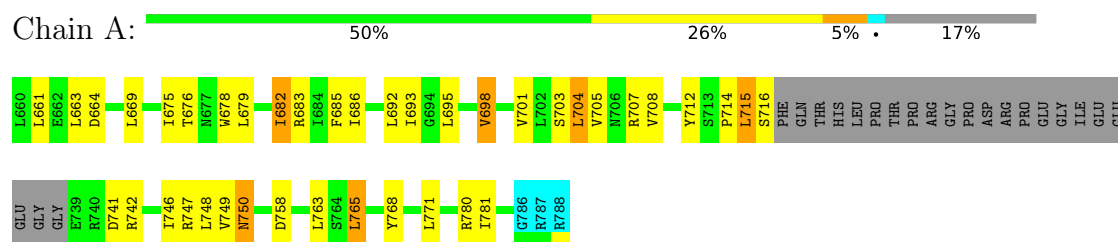


- Molecule 1: Envelope glycoprotein GP41



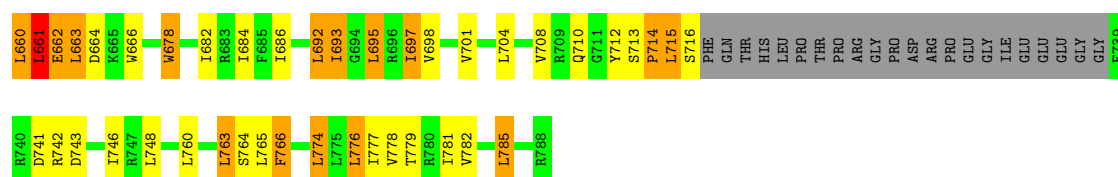
4.2.11 Score per residue for model 11

- Molecule 1: Envelope glycoprotein GP41

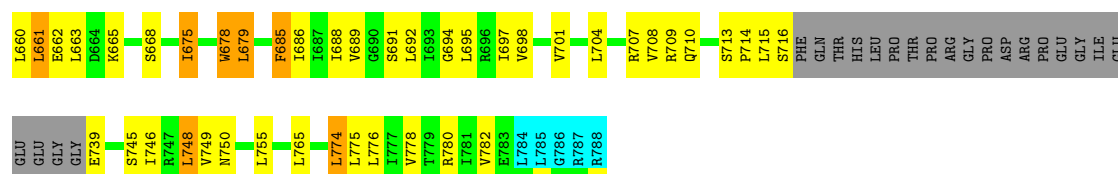


- Molecule 1: Envelope glycoprotein GP41



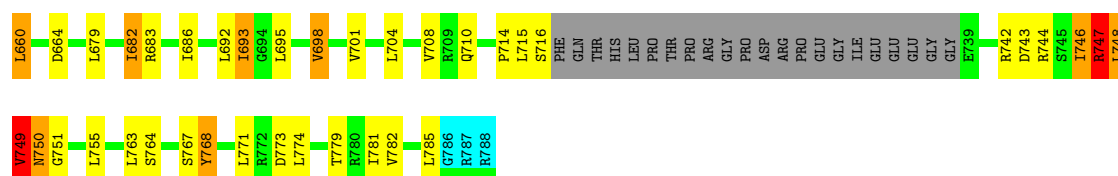


• Molecule 1: Envelope glycoprotein GP41

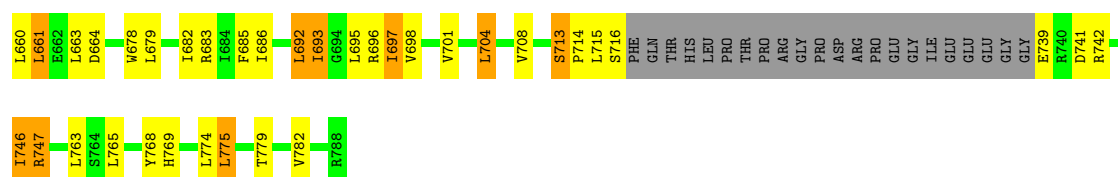


4.2.12 Score per residue for model 12

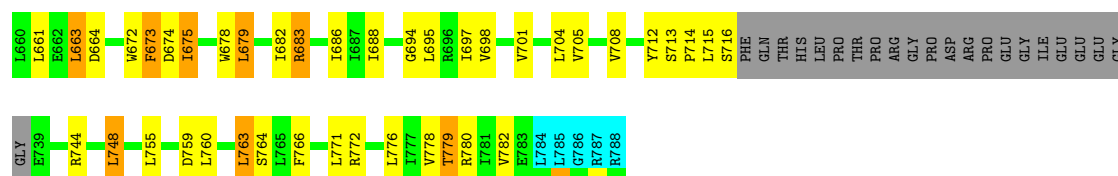
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

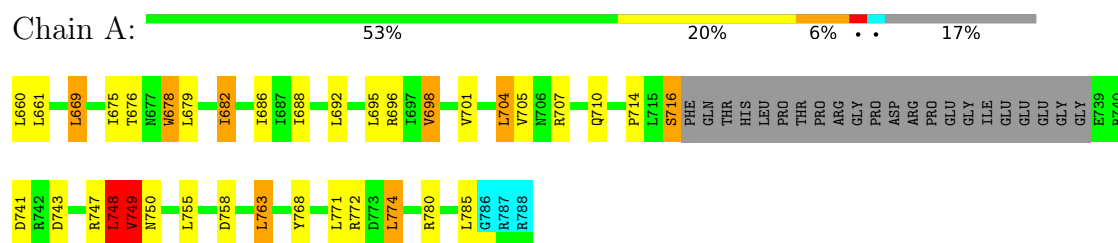


• Molecule 1: Envelope glycoprotein GP41

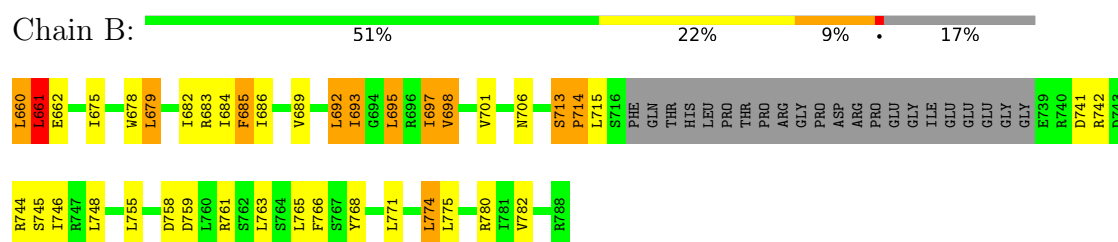


4.2.13 Score per residue for model 13

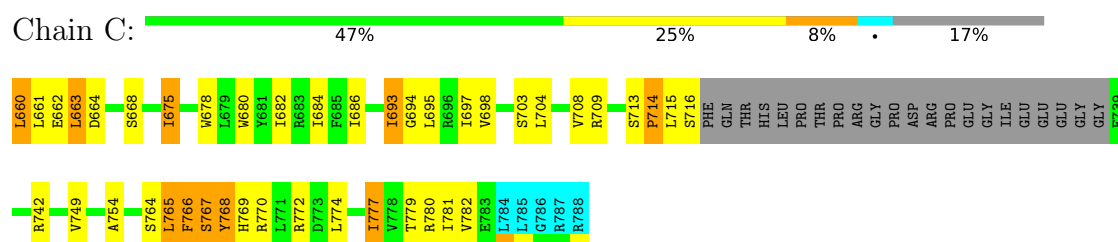
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

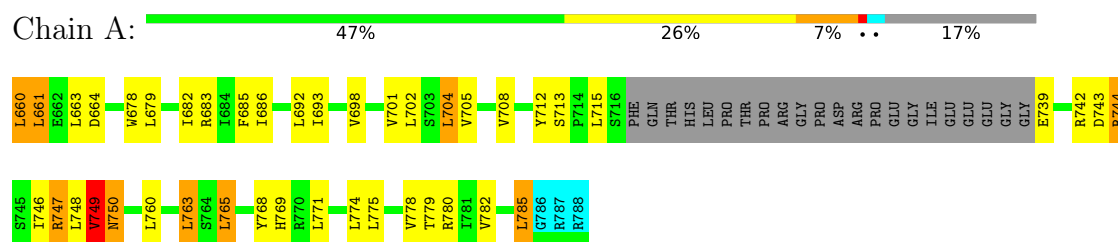


• Molecule 1: Envelope glycoprotein GP41



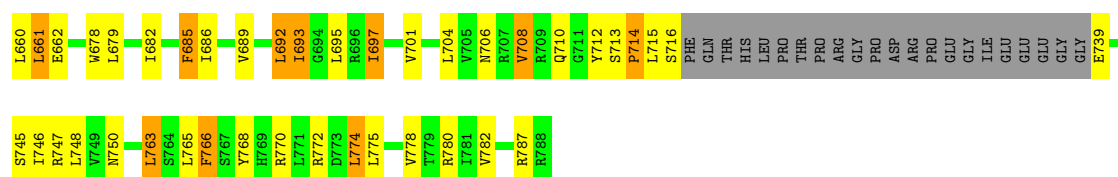
4.2.14 Score per residue for model 14

• Molecule 1: Envelope glycoprotein GP41



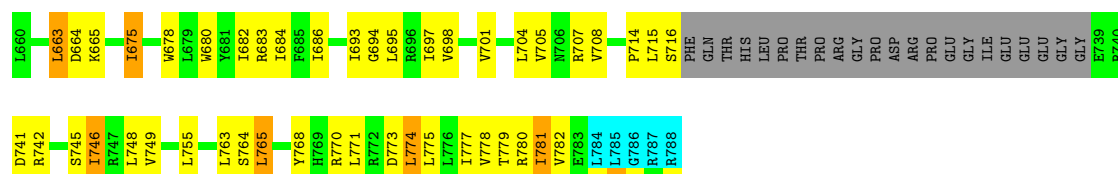
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

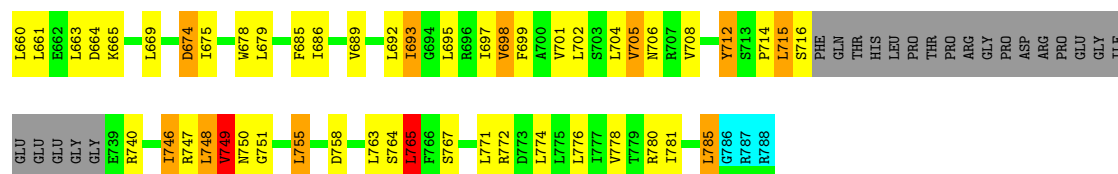
Chain C: 44% 30% 5% 17%



4.2.15 Score per residue for model 15

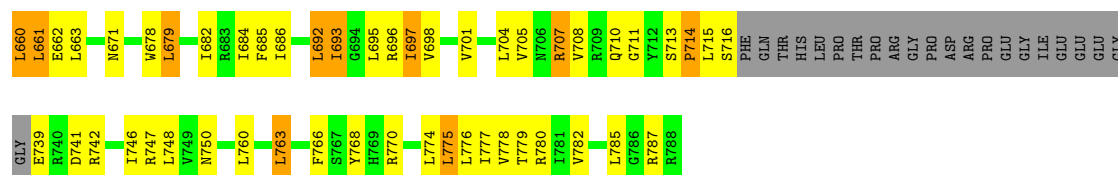
• Molecule 1: Envelope glycoprotein GP41

Chain A: 42% 29% 8% 17%



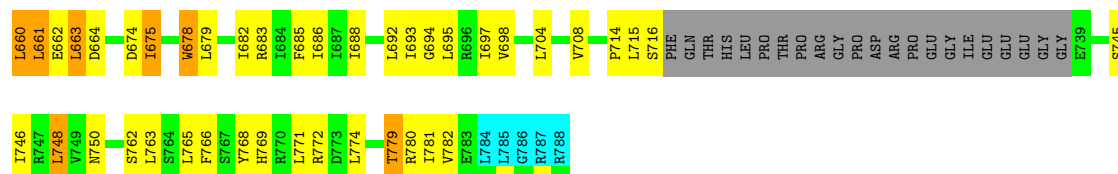
• Molecule 1: Envelope glycoprotein GP41

Chain B: 44% 31% 8% 17%



• Molecule 1: Envelope glycoprotein GP41

Chain C: 47% 27% 5% 17%



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 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
X-PLOR NIH	structure calculation	
X-PLOR NIH	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	520
Number of shifts mapped to atoms	427
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.88±0.02	0±0/899 (0.0± 0.0%)	1.15±0.02	1±1/1223 (0.1± 0.1%)
1	B	0.87±0.01	0±0/925 (0.0± 0.0%)	1.10±0.01	0±0/1253 (0.0± 0.0%)
1	C	0.85±0.02	0±0/883 (0.0± 0.0%)	1.10±0.01	0±0/1201 (0.0± 0.0%)
All	All	0.87	1/40605 (0.0%)	1.12	14/55155 (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	0.1±0.3
All	All	0	2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	749	VAL	CA-CB	5.02	1.59	1.54	8	1

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	749	VAL	N-CA-CB	-7.41	102.29	110.51	7	9
1	A	748	LEU	N-CA-C	-5.34	105.87	112.38	7	4
1	A	749	VAL	CB-CA-C	-5.30	105.10	111.88	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	707	ARG	Sidechain	1
1	A	747	ARG	Sidechain	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	879	924	919	25±5
1	B	906	953	948	28±4
1	C	863	902	897	26±5
All	All	39720	41685	41460	969

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HG23	1:B:746:ILE:HG23	0.86	1.47	8	1
1:A:686:ILE:HD12	1:C:686:ILE:HG21	0.81	1.52	9	12
1:A:705:VAL:HG22	1:A:748:LEU:HD11	0.80	1.53	13	1
1:B:781:ILE:HG23	1:C:746:ILE:HG23	0.79	1.52	4	2
1:A:686:ILE:HG21	1:B:686:ILE:HD12	0.78	1.55	15	12
1:A:774:LEU:HD22	1:A:777:ILE:HD11	0.77	1.55	8	1
1:B:785:LEU:HD23	1:C:750:ASN:ND2	0.75	1.96	9	4
1:A:779:THR:O	1:A:782:VAL:HG22	0.74	1.81	7	9
1:C:779:THR:O	1:C:782:VAL:HG22	0.73	1.83	8	10
1:A:748:LEU:O	1:A:748:LEU:HD13	0.73	1.84	5	8
1:A:669:LEU:HD23	1:A:676:THR:HG23	0.73	1.59	7	2
1:A:705:VAL:HG22	1:A:748:LEU:HD12	0.73	1.59	9	4
1:B:779:THR:O	1:B:782:VAL:HG22	0.71	1.85	9	10
1:A:758:ASP:OD1	1:B:715:LEU:HD22	0.71	1.86	15	2
1:C:759:ASP:O	1:C:763:LEU:HD22	0.71	1.85	7	1
1:B:742:ARG:O	1:B:746:ILE:HD12	0.71	1.85	12	1
1:A:746:ILE:HG22	1:C:781:ILE:HG21	0.70	1.62	14	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.70	1.86	12	14
1:B:682:ILE:HD12	1:B:683:ARG:N	0.69	2.02	1	6
1:A:678:TRP:O	1:A:682:ILE:HG23	0.69	1.86	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:777:ILE:HD13	1:A:778:VAL:N	0.68	2.02	7	2
1:A:746:ILE:O	1:A:749:VAL:HG22	0.68	1.88	11	1
1:A:663:LEU:HD23	1:B:660:LEU:N	0.68	2.03	8	1
1:A:693:ILE:O	1:A:693:ILE:HD13	0.68	1.89	15	2
1:A:768:TYR:CE1	1:A:771:LEU:HD23	0.68	2.23	8	1
1:A:781:ILE:HG21	1:B:746:ILE:CG2	0.68	2.19	10	2
1:A:705:VAL:HG22	1:A:748:LEU:HD23	0.68	1.64	3	1
1:C:775:LEU:O	1:C:778:VAL:HG22	0.68	1.88	7	4
1:B:663:LEU:HD12	1:C:660:LEU:HD23	0.67	1.66	3	1
1:C:682:ILE:HD12	1:C:683:ARG:N	0.67	2.05	14	9
1:C:675:ILE:O	1:C:675:ILE:HD13	0.67	1.90	9	10
1:A:682:ILE:HD12	1:A:683:ARG:N	0.67	2.04	14	5
1:C:742:ARG:O	1:C:746:ILE:HD12	0.67	1.90	14	5
1:A:705:VAL:HG23	1:A:748:LEU:HD12	0.66	1.66	15	1
1:A:778:VAL:O	1:A:781:ILE:HG22	0.66	1.90	10	2
1:B:686:ILE:HG21	1:C:686:ILE:HD12	0.66	1.67	7	9
1:B:781:ILE:HG23	1:C:746:ILE:CG2	0.66	2.21	4	1
1:A:705:VAL:CG2	1:A:748:LEU:HD12	0.66	2.21	14	3
1:A:758:ASP:CG	1:B:715:LEU:HD13	0.65	2.16	6	2
1:C:748:LEU:HD13	1:C:749:VAL:N	0.65	2.07	11	1
1:B:678:TRP:O	1:B:682:ILE:HG23	0.65	1.91	9	14
1:C:771:LEU:O	1:C:771:LEU:HD23	0.65	1.92	15	1
1:B:697:ILE:O	1:B:697:ILE:HD13	0.64	1.92	10	7
1:C:697:ILE:HD13	1:C:697:ILE:O	0.64	1.92	1	1
1:B:763:LEU:HA	1:B:774:LEU:HD22	0.64	1.69	3	1
1:B:778:VAL:O	1:B:781:ILE:HG22	0.64	1.91	10	1
1:B:771:LEU:HD23	1:B:771:LEU:O	0.64	1.93	2	2
1:A:660:LEU:N	1:C:663:LEU:HD23	0.63	2.08	15	8
1:A:746:ILE:HB	1:C:781:ILE:HG21	0.63	1.71	10	3
1:A:763:LEU:O	1:A:774:LEU:HD13	0.63	1.93	10	1
1:B:693:ILE:HD11	1:C:696:ARG:NE	0.63	2.07	7	3
1:B:660:LEU:C	1:B:661:LEU:HD22	0.63	2.19	11	4
1:B:675:ILE:HD13	1:B:675:ILE:O	0.62	1.95	7	1
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.62	1.53	12	3
1:A:743:ASP:HA	1:C:781:ILE:HD11	0.62	1.72	14	1
1:C:774:LEU:HD22	1:C:777:ILE:HD12	0.62	1.72	14	1
1:B:693:ILE:HD11	1:C:696:ARG:HE	0.62	1.52	10	2
1:C:745:SER:O	1:C:748:LEU:HD12	0.61	1.95	11	1
1:C:777:ILE:HG22	1:C:781:ILE:HD11	0.61	1.70	6	2
1:C:694:GLY:O	1:C:697:ILE:HG22	0.61	1.95	9	13
1:C:759:ASP:O	1:C:763:LEU:HD12	0.61	1.96	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HD11	1:B:746:ILE:CG2	0.61	2.25	11	1
1:C:705:VAL:HG13	1:C:748:LEU:HD21	0.61	1.72	12	2
1:A:758:ASP:OD2	1:B:715:LEU:HD22	0.61	1.95	13	2
1:C:778:VAL:O	1:C:781:ILE:HG22	0.61	1.94	14	2
1:C:678:TRP:O	1:C:682:ILE:HG23	0.60	1.96	15	12
1:B:781:ILE:HD12	1:C:746:ILE:HG13	0.60	1.72	5	1
1:B:758:ASP:CG	1:C:715:LEU:HD22	0.60	2.21	13	1
1:B:785:LEU:HD23	1:C:750:ASN:CG	0.60	2.22	10	2
1:B:774:LEU:O	1:B:778:VAL:HG23	0.60	1.97	11	4
1:A:780:ARG:NH2	1:A:784:LEU:HD21	0.60	2.12	7	1
1:B:694:GLY:O	1:B:697:ILE:HD12	0.60	1.97	7	1
1:A:777:ILE:HD12	1:A:778:VAL:N	0.59	2.12	5	1
1:C:763:LEU:C	1:C:763:LEU:HD22	0.59	2.22	12	1
1:B:775:LEU:HD13	1:B:775:LEU:O	0.59	1.97	6	10
1:A:746:ILE:CG2	1:C:781:ILE:HG21	0.59	2.27	14	1
1:C:777:ILE:HG22	1:C:781:ILE:CD1	0.59	2.27	6	2
1:A:693:ILE:HD12	1:A:693:ILE:O	0.59	1.97	8	4
1:C:663:LEU:HD22	1:C:663:LEU:O	0.59	1.96	14	4
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.59	1.75	5	1
1:A:774:LEU:HD12	1:B:742:ARG:NE	0.59	2.13	9	2
1:B:763:LEU:O	1:B:774:LEU:HD13	0.59	1.97	14	3
1:B:763:LEU:O	1:B:774:LEU:HD22	0.59	1.97	11	2
1:A:755:LEU:HD22	1:A:755:LEU:O	0.59	1.97	15	1
1:A:704:LEU:HD23	1:A:707:ARG:HD2	0.59	1.75	8	1
1:C:663:LEU:HD13	1:C:664:ASP:N	0.58	2.13	1	8
1:C:774:LEU:HD13	1:C:774:LEU:O	0.58	1.99	10	4
1:C:763:LEU:HD13	1:C:764:SER:H	0.58	1.57	12	1
1:B:686:ILE:CG2	1:C:686:ILE:HD12	0.57	2.28	7	9
1:C:660:LEU:N	1:C:660:LEU:HD13	0.57	2.14	4	2
1:A:675:ILE:HD13	1:A:675:ILE:O	0.57	1.99	8	2
1:C:675:ILE:HD13	1:C:678:TRP:CZ3	0.57	2.33	8	1
1:C:768:TYR:O	1:C:770:ARG:N	0.57	2.37	13	1
1:B:710:GLN:O	1:B:715:LEU:HD11	0.57	1.98	15	1
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.57	1.76	10	4
1:A:742:ARG:O	1:A:746:ILE:HD12	0.57	1.99	1	4
1:B:785:LEU:HD23	1:C:750:ASN:HD22	0.57	1.57	5	2
1:C:748:LEU:C	1:C:748:LEU:HD22	0.57	2.24	11	1
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.57	2.35	7	1
1:A:704:LEU:HD22	1:B:712:TYR:O	0.57	1.99	8	1
1:B:781:ILE:O	1:B:785:LEU:HD12	0.57	1.99	4	1
1:B:715:LEU:O	1:B:715:LEU:HD23	0.56	2.00	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:763:LEU:HD23	1:C:764:SER:H	0.56	1.60	7	1
1:C:693:ILE:C	1:C:693:ILE:HD13	0.56	2.25	13	1
1:A:763:LEU:HA	1:A:774:LEU:HD22	0.56	1.77	3	3
1:B:781:ILE:HG21	1:C:746:ILE:CG2	0.56	2.31	11	2
1:A:749:VAL:HG23	1:A:750:ASN:ND2	0.56	2.15	11	1
1:B:785:LEU:HD23	1:C:750:ASN:HB2	0.56	1.75	1	1
1:A:663:LEU:HD12	1:B:660:LEU:N	0.56	2.15	9	4
1:A:746:ILE:HD12	1:C:781:ILE:CD1	0.56	2.30	5	1
1:A:749:VAL:HG21	1:C:782:VAL:HG12	0.56	1.77	11	1
1:C:685:PHE:O	1:C:689:VAL:HG23	0.56	2.01	4	3
1:A:701:VAL:O	1:A:705:VAL:HG23	0.56	2.01	13	2
1:C:698:VAL:O	1:C:701:VAL:HG22	0.56	2.01	11	1
1:B:785:LEU:HD13	1:C:750:ASN:HD21	0.56	1.61	4	1
1:C:763:LEU:HD23	1:C:764:SER:N	0.56	2.15	7	1
1:A:682:ILE:HD12	1:A:683:ARG:H	0.55	1.62	5	4
1:C:693:ILE:HD12	1:C:693:ILE:O	0.55	2.01	5	1
1:C:764:SER:HB3	1:C:771:LEU:HD12	0.55	1.78	7	1
1:A:748:LEU:C	1:A:748:LEU:HD13	0.55	2.26	13	1
1:A:763:LEU:O	1:A:774:LEU:HD22	0.55	2.01	13	1
1:B:693:ILE:C	1:B:693:ILE:HD13	0.55	2.26	7	2
1:A:715:LEU:HD23	1:C:758:ASP:OD2	0.55	2.01	10	1
1:A:705:VAL:HG22	1:A:748:LEU:CD1	0.55	2.29	13	1
1:A:748:LEU:O	1:A:748:LEU:HD22	0.55	2.01	13	1
1:B:715:LEU:O	1:B:716:SER:C	0.55	2.49	8	11
1:C:695:LEU:O	1:C:698:VAL:HG12	0.55	2.00	15	11
1:B:710:GLN:O	1:B:715:LEU:HD12	0.55	2.01	14	3
1:B:692:LEU:HD12	1:B:693:ILE:N	0.55	2.17	3	12
1:B:785:LEU:HD22	1:C:750:ASN:CG	0.55	2.27	4	1
1:B:693:ILE:HD12	1:B:693:ILE:O	0.54	2.02	10	2
1:C:715:LEU:O	1:C:716:SER:C	0.54	2.50	7	9
1:A:693:ILE:HD13	1:A:693:ILE:C	0.54	2.27	1	2
1:A:704:LEU:HD11	1:B:712:TYR:O	0.54	2.03	14	4
1:C:763:LEU:HD13	1:C:764:SER:N	0.54	2.17	12	1
1:A:780:ARG:NH2	1:A:784:LEU:HD11	0.54	2.18	7	1
1:B:697:ILE:HD13	1:B:698:VAL:H	0.54	1.63	7	1
1:B:774:LEU:HD11	1:C:742:ARG:CZ	0.54	2.32	13	1
1:A:749:VAL:HG12	1:A:750:ASN:ND2	0.54	2.18	12	8
1:A:747:ARG:NE	1:C:782:VAL:HA	0.54	2.18	2	1
1:A:746:ILE:HD12	1:C:781:ILE:HD12	0.54	1.78	5	1
1:A:746:ILE:HG22	1:C:781:ILE:HD13	0.54	1.79	8	1
1:B:663:LEU:CD1	1:C:660:LEU:HD22	0.54	2.32	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:777:ILE:HG22	1:C:781:ILE:HD12	0.54	1.78	14	1
1:C:660:LEU:HD22	1:C:660:LEU:C	0.53	2.27	3	1
1:A:763:LEU:HA	1:A:774:LEU:HD13	0.53	1.78	12	4
1:A:774:LEU:HD11	1:B:742:ARG:NH2	0.53	2.18	3	1
1:B:785:LEU:HD22	1:C:750:ASN:ND2	0.53	2.18	4	2
1:A:781:ILE:HG21	1:B:746:ILE:HG21	0.53	1.80	10	2
1:A:774:LEU:CD1	1:A:777:ILE:HD11	0.53	2.34	5	1
1:B:695:LEU:O	1:B:698:VAL:HG12	0.53	2.02	1	9
1:A:748:LEU:HD23	1:A:748:LEU:O	0.53	2.04	8	1
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.53	1.63	5	1
1:C:773:ASP:OD2	1:C:774:LEU:HD22	0.53	2.04	7	1
1:B:781:ILE:HG21	1:C:746:ILE:HG22	0.53	1.79	11	1
1:B:764:SER:C	1:B:765:LEU:HD12	0.53	2.29	3	1
1:B:705:VAL:HG13	1:B:748:LEU:CD2	0.53	2.34	4	1
1:A:785:LEU:HD22	1:B:750:ASN:ND2	0.52	2.19	9	3
1:A:774:LEU:HD13	1:A:774:LEU:O	0.52	2.05	8	1
1:A:781:ILE:HD11	1:B:746:ILE:HB	0.52	1.80	11	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.52	2.04	14	2
1:B:705:VAL:HG22	1:B:748:LEU:HD23	0.52	1.80	15	1
1:B:661:LEU:N	1:B:661:LEU:HD22	0.52	2.20	10	9
1:A:758:ASP:CB	1:B:715:LEU:HD13	0.52	2.34	6	2
1:B:708:VAL:HG11	1:B:748:LEU:HD21	0.52	1.82	14	1
1:A:763:LEU:HD23	1:A:771:LEU:HD11	0.52	1.80	5	2
1:A:675:ILE:CG1	1:A:679:LEU:HD23	0.52	2.35	13	1
1:B:708:VAL:HG11	1:B:748:LEU:HD11	0.52	1.82	5	1
1:C:745:SER:O	1:C:748:LEU:HD22	0.52	2.05	8	1
1:B:785:LEU:HD22	1:C:747:ARG:HA	0.52	1.81	9	1
1:A:774:LEU:O	1:A:778:VAL:HG13	0.51	2.05	2	1
1:B:660:LEU:HG	1:B:661:LEU:HD22	0.51	1.82	6	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.51	2.31	7	1
1:A:781:ILE:CD1	1:B:746:ILE:HD13	0.51	2.35	12	1
1:A:785:LEU:HD23	1:B:750:ASN:ND2	0.51	2.21	8	3
1:B:748:LEU:O	1:B:748:LEU:HD23	0.51	2.05	6	1
1:C:748:LEU:HD12	1:C:748:LEU:O	0.51	2.05	12	1
1:C:777:ILE:O	1:C:781:ILE:HG13	0.51	2.05	2	1
1:B:663:LEU:HD13	1:C:660:LEU:HD22	0.51	1.83	10	2
1:C:749:VAL:HG12	1:C:750:ASN:ND2	0.51	2.21	9	1
1:C:660:LEU:C	1:C:660:LEU:HD12	0.51	2.31	9	3
1:C:755:LEU:C	1:C:755:LEU:HD13	0.51	2.31	10	2
1:A:758:ASP:HB3	1:B:715:LEU:HD13	0.51	1.82	15	1
1:A:693:ILE:C	1:A:693:ILE:HD13	0.50	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:774:LEU:HD22	1:C:777:ILE:CD1	0.50	2.36	14	1
1:A:777:ILE:HD11	1:B:742:ARG:HH11	0.50	1.66	1	1
1:C:755:LEU:C	1:C:755:LEU:HD23	0.50	2.31	5	10
1:A:774:LEU:HD12	1:A:777:ILE:HD11	0.50	1.81	5	1
1:B:748:LEU:C	1:B:748:LEU:HD23	0.50	2.31	2	1
1:C:663:LEU:C	1:C:663:LEU:HD13	0.50	2.32	3	5
1:C:774:LEU:C	1:C:774:LEU:HD13	0.50	2.32	8	2
1:C:663:LEU:HD22	1:C:663:LEU:C	0.50	2.32	14	3
1:B:755:LEU:C	1:B:755:LEU:HD23	0.50	2.31	1	3
1:A:748:LEU:HD13	1:B:714:PRO:CG	0.50	2.37	4	1
1:A:669:LEU:CD2	1:A:676:THR:HG23	0.50	2.34	7	1
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.50	1.82	13	1
1:C:748:LEU:O	1:C:748:LEU:HD23	0.49	2.06	15	2
1:B:675:ILE:HG13	1:B:679:LEU:HD23	0.49	1.84	6	1
1:B:785:LEU:HD13	1:C:750:ASN:ND2	0.49	2.23	4	1
1:A:749:VAL:HG23	1:A:750:ASN:HD22	0.49	1.66	11	1
1:C:774:LEU:HD13	1:C:777:ILE:HG22	0.49	1.85	1	1
1:A:781:ILE:HG21	1:B:746:ILE:HG23	0.49	1.84	10	2
1:A:746:ILE:HG12	1:C:778:VAL:HG12	0.49	1.85	12	2
1:A:704:LEU:HD22	1:B:707:ARG:NH2	0.49	2.23	6	1
1:A:784:LEU:N	1:A:784:LEU:HD13	0.49	2.23	7	1
1:A:742:ARG:CZ	1:C:774:LEU:HD21	0.49	2.38	11	1
1:A:663:LEU:C	1:A:663:LEU:HD13	0.49	2.31	8	1
1:A:705:VAL:HG23	1:A:748:LEU:CB	0.49	2.38	8	1
1:A:776:LEU:C	1:A:776:LEU:HD13	0.49	2.32	8	1
1:A:695:LEU:HD23	1:A:695:LEU:O	0.49	2.07	2	1
1:B:748:LEU:C	1:B:748:LEU:HD12	0.49	2.33	9	2
1:A:771:LEU:O	1:A:771:LEU:HD12	0.49	2.08	8	1
1:A:781:ILE:HD11	1:B:746:ILE:CB	0.49	2.37	11	1
1:A:690:GLY:O	1:A:693:ILE:HG23	0.49	2.07	7	1
1:B:697:ILE:HD13	1:B:698:VAL:N	0.49	2.23	7	1
1:B:765:LEU:C	1:B:765:LEU:HD13	0.49	2.33	8	1
1:A:747:ARG:C	1:A:749:VAL:N	0.48	2.69	7	9
1:B:694:GLY:O	1:B:697:ILE:HG22	0.48	2.08	2	3
1:C:708:VAL:HG12	1:C:748:LEU:HD11	0.48	1.85	10	1
1:A:748:LEU:HD13	1:A:748:LEU:C	0.48	2.32	15	3
1:A:748:LEU:HD13	1:B:714:PRO:HG3	0.48	1.83	4	2
1:B:705:VAL:HG22	1:B:748:LEU:HD13	0.48	1.85	4	1
1:B:781:ILE:CG2	1:C:746:ILE:HG23	0.48	2.39	5	1
1:B:777:ILE:HD12	1:B:778:VAL:N	0.48	2.23	6	1
1:A:743:ASP:O	1:C:781:ILE:HG23	0.48	2.09	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:716:SER:HA	1:C:754:ALA:HB1	0.48	1.84	13	1
1:C:767:SER:O	1:C:768:TYR:C	0.48	2.55	13	1
1:A:746:ILE:CG2	1:C:781:ILE:HD12	0.48	2.38	2	1
1:B:661:LEU:HD22	1:B:661:LEU:N	0.48	2.24	13	1
1:C:679:LEU:HD13	1:C:679:LEU:O	0.48	2.09	4	2
1:B:755:LEU:C	1:B:755:LEU:HD13	0.48	2.34	13	2
1:B:661:LEU:HD12	1:B:666:TRP:CE2	0.48	2.44	11	1
1:A:675:ILE:HG12	1:A:679:LEU:HD23	0.48	1.84	13	1
1:A:755:LEU:C	1:A:755:LEU:HD23	0.48	2.34	8	6
1:B:675:ILE:HD11	1:B:678:TRP:CE3	0.48	2.43	7	1
1:A:675:ILE:HG13	1:A:679:LEU:HD23	0.48	1.84	15	2
1:A:747:ARG:NH1	1:C:781:ILE:HG22	0.48	2.24	5	1
1:B:679:LEU:HD13	1:B:679:LEU:O	0.48	2.08	10	3
1:A:743:ASP:O	1:C:781:ILE:HG21	0.47	2.09	2	1
1:B:663:LEU:C	1:B:663:LEU:HD23	0.47	2.34	8	2
1:A:743:ASP:CB	1:C:781:ILE:HD12	0.47	2.38	13	1
1:A:780:ARG:HH21	1:A:784:LEU:HD21	0.47	1.69	7	1
1:C:764:SER:CB	1:C:771:LEU:HD12	0.47	2.39	9	2
1:C:765:LEU:N	1:C:765:LEU:HD22	0.47	2.24	8	1
1:A:748:LEU:HD22	1:A:751:GLY:HA3	0.47	1.85	15	2
1:B:692:LEU:HD12	1:B:693:ILE:H	0.47	1.70	6	10
1:C:663:LEU:HD13	1:C:663:LEU:C	0.47	2.34	9	6
1:B:755:LEU:HD21	1:C:710:GLN:NE2	0.47	2.25	4	1
1:B:765:LEU:HD13	1:B:765:LEU:O	0.47	2.09	8	1
1:A:746:ILE:HG21	1:C:781:ILE:HD12	0.47	1.85	2	1
1:A:774:LEU:HD11	1:B:742:ARG:CZ	0.47	2.40	3	1
1:A:705:VAL:HG23	1:A:748:LEU:CD1	0.47	2.39	8	1
1:B:774:LEU:HD12	1:C:742:ARG:HE	0.47	1.68	9	1
1:B:760:LEU:C	1:B:760:LEU:HD13	0.47	2.34	7	1
1:B:689:VAL:O	1:B:692:LEU:HD11	0.47	2.10	8	1
1:C:748:LEU:HD22	1:C:748:LEU:O	0.47	2.10	11	1
1:A:746:ILE:O	1:A:749:VAL:HB	0.47	2.10	6	4
1:B:693:ILE:C	1:B:693:ILE:HD12	0.47	2.35	4	6
1:A:715:LEU:H	1:A:715:LEU:HD23	0.47	1.69	7	2
1:B:675:ILE:HD11	1:B:679:LEU:HD23	0.47	1.86	10	1
1:B:776:LEU:O	1:B:779:THR:HG22	0.47	2.09	15	2
1:B:775:LEU:C	1:B:775:LEU:HD13	0.47	2.35	14	1
1:A:747:ARG:CZ	1:A:750:ASN:CG	0.47	2.88	2	1
1:A:774:LEU:HD12	1:B:742:ARG:HE	0.47	1.70	9	1
1:B:669:LEU:HD12	1:B:675:ILE:CG2	0.47	2.40	8	1
1:B:690:GLY:O	1:B:693:ILE:HG23	0.47	2.09	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:695:LEU:O	1:C:695:LEU:HD23	0.47	2.10	11	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.47	2.10	2	1
1:A:748:LEU:HD21	1:B:714:PRO:CG	0.46	2.40	7	1
1:A:746:ILE:HD13	1:C:781:ILE:CD1	0.46	2.40	15	1
1:C:777:ILE:CG2	1:C:781:ILE:HD11	0.46	2.40	6	2
1:A:713:SER:OG	1:C:708:VAL:HG23	0.46	2.09	7	1
1:B:675:ILE:HD12	1:B:675:ILE:O	0.46	2.10	10	1
1:A:707:ARG:HH21	1:A:708:VAL:HG23	0.46	1.70	1	1
1:C:661:LEU:HD12	1:C:661:LEU:N	0.46	2.25	15	3
1:C:748:LEU:C	1:C:748:LEU:HD12	0.46	2.35	4	1
1:A:703:SER:OG	1:C:700:ALA:HB1	0.46	2.09	10	1
1:B:713:SER:O	1:B:714:PRO:C	0.46	2.59	15	13
1:A:678:TRP:C	1:A:678:TRP:CD1	0.46	2.94	9	2
1:B:708:VAL:CG1	1:B:748:LEU:HD11	0.46	2.41	8	1
1:A:693:ILE:HG22	1:C:693:ILE:HG21	0.46	1.86	2	1
1:C:708:VAL:CG1	1:C:748:LEU:HD11	0.46	2.40	10	1
1:A:747:ARG:HG3	1:A:747:ARG:O	0.46	2.11	7	1
1:C:778:VAL:O	1:C:782:VAL:HG13	0.46	2.10	11	1
1:B:763:LEU:HA	1:B:774:LEU:HD13	0.45	1.87	7	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.45	2.11	13	2
1:B:686:ILE:HG22	1:C:686:ILE:HD12	0.45	1.88	2	1
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.45	2.26	5	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.45	2.12	12	2
1:B:708:VAL:CG1	1:B:748:LEU:HD12	0.45	2.41	1	1
1:A:693:ILE:HG13	1:B:693:ILE:HG22	0.45	1.89	3	2
1:C:765:LEU:O	1:C:766:PHE:C	0.45	2.59	6	2
1:C:763:LEU:HD23	1:C:763:LEU:C	0.45	2.36	10	3
1:B:705:VAL:HG22	1:B:748:LEU:HD11	0.45	1.88	2	1
1:A:765:LEU:C	1:A:765:LEU:HD23	0.45	2.36	3	2
1:B:663:LEU:CD1	1:C:660:LEU:HD23	0.45	2.39	3	1
1:C:776:LEU:C	1:C:776:LEU:HD23	0.45	2.36	6	1
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.45	2.37	7	1
1:A:715:LEU:HD23	1:A:716:SER:N	0.45	2.27	11	2
1:A:696:ARG:CG	1:C:693:ILE:HD11	0.45	2.42	13	1
1:A:706:ASN:O	1:A:710:GLN:HB2	0.45	2.12	5	2
1:A:743:ASP:HA	1:C:781:ILE:HD13	0.45	1.88	2	1
1:A:743:ASP:HB3	1:C:781:ILE:HD12	0.45	1.87	13	1
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.45	2.42	14	1
1:C:713:SER:O	1:C:714:PRO:C	0.45	2.59	13	8
1:A:695:LEU:O	1:A:698:VAL:HG12	0.45	2.12	4	3
1:B:781:ILE:HG23	1:C:746:ILE:HG13	0.45	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:705:VAL:HA	1:B:748:LEU:HD13	0.45	1.88	8	1
1:A:781:ILE:CG2	1:B:746:ILE:HG23	0.45	2.42	7	1
1:A:747:ARG:NE	1:A:750:ASN:ND2	0.45	2.64	2	1
1:A:704:LEU:HD13	1:A:707:ARG:NH2	0.45	2.27	11	2
1:A:765:LEU:HD22	1:A:765:LEU:O	0.45	2.12	11	1
1:B:684:ILE:HD12	1:B:684:ILE:N	0.45	2.25	3	10
1:B:771:LEU:C	1:B:771:LEU:HD23	0.45	2.37	1	3
1:A:758:ASP:HB3	1:B:710:GLN:CB	0.45	2.42	3	1
1:A:693:ILE:HD11	1:B:696:ARG:HG2	0.45	1.88	7	1
1:B:669:LEU:HD12	1:B:675:ILE:HG21	0.45	1.89	8	1
1:C:777:ILE:O	1:C:781:ILE:HG12	0.45	2.12	13	1
1:B:663:LEU:CD1	1:C:660:LEU:HD13	0.45	2.42	15	1
1:A:669:LEU:HD22	1:A:676:THR:OG1	0.44	2.13	8	1
1:B:715:LEU:HD22	1:B:715:LEU:N	0.44	2.27	8	1
1:B:697:ILE:HD13	1:B:697:ILE:C	0.44	2.37	15	4
1:B:682:ILE:HD12	1:B:683:ARG:H	0.44	1.70	5	1
1:A:765:LEU:C	1:A:765:LEU:HD13	0.44	2.37	9	2
1:A:704:LEU:HD22	1:A:707:ARG:NH1	0.44	2.27	13	1
1:B:771:LEU:HD23	1:B:771:LEU:C	0.44	2.37	2	1
1:C:661:LEU:HD22	1:C:661:LEU:N	0.44	2.26	9	1
1:C:693:ILE:HD12	1:C:693:ILE:C	0.44	2.37	5	2
1:C:715:LEU:HD22	1:C:715:LEU:N	0.44	2.27	11	1
1:B:672:TRP:O	1:B:674:ASP:N	0.44	2.50	5	1
1:A:660:LEU:CB	1:C:663:LEU:HD21	0.44	2.42	3	1
1:A:705:VAL:HG23	1:A:748:LEU:HD13	0.44	1.90	8	1
1:A:748:LEU:HD23	1:B:714:PRO:HB3	0.44	1.90	9	1
1:A:748:LEU:HD12	1:A:751:GLY:HA3	0.44	1.90	3	1
1:B:774:LEU:HD11	1:C:742:ARG:NE	0.44	2.28	3	1
1:C:675:ILE:HD12	1:C:679:LEU:HD12	0.44	1.90	11	1
1:A:713:SER:O	1:A:714:PRO:C	0.44	2.60	2	2
1:C:660:LEU:HD23	1:C:660:LEU:N	0.44	2.28	5	1
1:B:660:LEU:N	1:B:660:LEU:HD12	0.44	2.27	7	1
1:A:765:LEU:HD22	1:A:765:LEU:C	0.44	2.37	11	1
1:A:660:LEU:CB	1:C:663:LEU:HD23	0.44	2.42	12	2
1:C:742:ARG:O	1:C:746:ILE:HD13	0.44	2.13	6	2
1:B:663:LEU:HD12	1:C:660:LEU:HD13	0.44	1.90	6	2
1:A:765:LEU:HD23	1:B:739:GLU:CD	0.44	2.38	15	1
1:C:678:TRP:C	1:C:678:TRP:CD1	0.43	2.96	5	1
1:A:661:LEU:N	1:A:661:LEU:HD12	0.43	2.27	7	1
1:A:763:LEU:HB2	1:A:771:LEU:HD13	0.43	1.90	8	1
1:A:768:TYR:CE1	1:A:771:LEU:HD22	0.43	2.48	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:663:LEU:C	1:C:663:LEU:HD23	0.43	2.37	4	2
1:C:771:LEU:C	1:C:771:LEU:HD23	0.43	2.37	7	2
1:A:669:LEU:HD23	1:A:676:THR:OG1	0.43	2.13	13	1
1:B:663:LEU:HD23	1:B:664:ASP:N	0.43	2.28	11	3
1:C:761:ARG:O	1:C:765:LEU:HD13	0.43	2.13	8	1
1:B:696:ARG:N	1:B:696:ARG:HD2	0.43	2.28	9	1
1:B:768:TYR:CE2	1:B:771:LEU:HD13	0.43	2.48	1	1
1:B:758:ASP:OD2	1:C:715:LEU:HD23	0.43	2.14	10	1
1:B:705:VAL:HG13	1:B:748:LEU:HD22	0.43	1.91	4	1
1:A:775:LEU:O	1:A:778:VAL:HG22	0.43	2.13	8	1
1:A:693:ILE:HD11	1:B:696:ARG:CG	0.43	2.43	10	1
1:A:704:LEU:HD13	1:A:707:ARG:HH22	0.43	1.73	11	1
1:A:684:ILE:HD12	1:A:684:ILE:N	0.43	2.29	4	3
1:A:762:SER:O	1:A:774:LEU:HD13	0.43	2.13	9	1
1:A:705:VAL:CG2	1:A:748:LEU:HD23	0.43	2.40	3	1
1:C:679:LEU:HD23	1:C:679:LEU:O	0.43	2.14	5	2
1:A:784:LEU:HD22	1:A:784:LEU:H	0.43	1.74	7	1
1:A:715:LEU:O	1:A:716:SER:C	0.43	2.62	10	1
1:A:673:PHE:O	1:A:673:PHE:CG	0.43	2.71	3	1
1:C:675:ILE:HD11	1:C:678:TRP:CE3	0.43	2.48	13	3
1:A:781:ILE:HD11	1:B:746:ILE:HG21	0.43	1.90	11	1
1:C:669:LEU:HD22	1:C:669:LEU:N	0.43	2.29	2	2
1:A:660:LEU:HB2	1:C:663:LEU:HD21	0.43	1.91	3	1
1:C:746:ILE:O	1:C:749:VAL:HG23	0.43	2.14	10	1
1:A:768:TYR:CZ	1:A:771:LEU:HD22	0.43	2.49	14	1
1:B:693:ILE:HD13	1:B:693:ILE:O	0.42	2.14	5	1
1:A:748:LEU:HD23	1:B:714:PRO:HG3	0.42	1.91	10	1
1:A:705:VAL:HG13	1:A:748:LEU:HD12	0.42	1.91	13	1
1:A:777:ILE:HD11	1:B:742:ARG:NH1	0.42	2.29	1	1
1:C:774:LEU:HD13	1:C:774:LEU:C	0.42	2.38	10	1
1:B:774:LEU:HD11	1:C:742:ARG:NH2	0.42	2.30	13	1
1:A:663:LEU:C	1:A:663:LEU:HD23	0.42	2.39	14	1
1:B:775:LEU:HD13	1:B:775:LEU:C	0.42	2.39	7	2
1:A:775:LEU:HD23	1:A:775:LEU:C	0.42	2.40	4	1
1:B:774:LEU:C	1:B:774:LEU:HD12	0.42	2.39	4	1
1:A:768:TYR:CE1	1:A:771:LEU:HD13	0.42	2.49	11	1
1:C:684:ILE:N	1:C:684:ILE:HD12	0.42	2.28	13	1
1:C:678:TRP:CD1	1:C:678:TRP:C	0.42	2.98	9	5
1:B:763:LEU:HG	1:B:774:LEU:HD22	0.42	1.90	10	1
1:B:782:VAL:HG11	1:C:749:VAL:HG11	0.42	1.91	14	2
1:C:764:SER:OG	1:C:771:LEU:HD12	0.42	2.14	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:755:LEU:HD21	1:B:710:GLN:NE2	0.42	2.29	7	1
1:C:675:ILE:HD13	1:C:675:ILE:C	0.42	2.39	5	2
1:B:706:ASN:O	1:B:710:GLN:HG2	0.42	2.15	14	2
1:A:749:VAL:HG23	1:A:750:ASN:N	0.42	2.30	11	1
1:C:705:VAL:HG13	1:C:748:LEU:HD11	0.42	1.92	12	1
1:B:689:VAL:O	1:B:692:LEU:CD1	0.42	2.67	14	3
1:A:746:ILE:O	1:A:749:VAL:CG2	0.42	2.68	8	1
1:A:712:TYR:CD1	1:C:707:ARG:CZ	0.42	3.03	9	1
1:C:763:LEU:HD21	1:C:771:LEU:HD12	0.42	1.91	12	1
1:A:713:SER:HA	1:C:708:VAL:HG21	0.42	1.91	14	1
1:A:685:PHE:O	1:A:689:VAL:HG23	0.42	2.15	15	1
1:B:682:ILE:N	1:B:682:ILE:HD13	0.41	2.30	10	2
1:A:697:ILE:O	1:A:697:ILE:HD13	0.41	2.15	9	1
1:C:684:ILE:O	1:C:688:ILE:HD13	0.41	2.15	2	1
1:C:705:VAL:HG13	1:C:748:LEU:HD13	0.41	1.92	2	1
1:A:747:ARG:CD	1:C:782:VAL:HA	0.41	2.45	13	1
1:A:758:ASP:HB3	1:B:710:GLN:HB2	0.41	1.92	1	2
1:C:704:LEU:HD13	1:C:704:LEU:O	0.41	2.15	1	1
1:C:775:LEU:O	1:C:778:VAL:HG12	0.41	2.15	2	1
1:B:778:VAL:HG23	1:C:746:ILE:CG1	0.41	2.45	6	1
1:B:689:VAL:O	1:B:692:LEU:HD12	0.41	2.14	9	1
1:C:768:TYR:CZ	1:C:771:LEU:HD13	0.41	2.50	15	1
1:A:693:ILE:HG22	1:C:693:ILE:HB	0.41	1.92	5	1
1:B:774:LEU:HG	1:B:777:ILE:HD11	0.41	1.92	11	1
1:C:672:TRP:O	1:C:673:PHE:C	0.41	2.63	12	1
1:A:712:TYR:CZ	1:C:707:ARG:NH1	0.41	2.89	14	1
1:A:776:LEU:HD12	1:A:776:LEU:N	0.41	2.30	15	1
1:B:669:LEU:HD22	1:B:669:LEU:N	0.41	2.30	8	1
1:B:706:ASN:O	1:B:710:GLN:HB2	0.41	2.15	8	1
1:B:707:ARG:O	1:B:711:GLY:C	0.41	2.64	15	2
1:A:678:TRP:CD1	1:A:678:TRP:C	0.41	2.99	15	2
1:B:678:TRP:CD1	1:B:678:TRP:C	0.41	2.98	15	1
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.41	2.50	1	1
1:A:746:ILE:CD1	1:C:781:ILE:HD12	0.41	2.46	5	1
1:A:693:ILE:HG22	1:C:693:ILE:CB	0.41	2.46	5	1
1:C:764:SER:O	1:C:765:LEU:HB3	0.41	2.16	5	1
1:A:768:TYR:CE2	1:A:771:LEU:HD13	0.41	2.50	12	1
1:A:763:LEU:HB2	1:A:771:LEU:HD12	0.41	1.92	14	1
1:B:755:LEU:HD21	1:C:710:GLN:HE22	0.41	1.76	1	1
1:B:762:SER:O	1:B:774:LEU:HD22	0.41	2.16	2	1
1:A:705:VAL:HG22	1:A:748:LEU:CD2	0.41	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:715:LEU:O	1:C:715:LEU:HD23	0.41	2.15	4	1
1:A:713:SER:CB	1:C:708:VAL:HG23	0.41	2.46	7	1
1:C:697:ILE:HD13	1:C:697:ILE:C	0.41	2.41	1	1
1:B:745:SER:O	1:B:748:LEU:HD23	0.41	2.15	13	2
1:C:748:LEU:HD13	1:C:748:LEU:O	0.41	2.16	1	1
1:A:684:ILE:O	1:A:688:ILE:HD13	0.41	2.16	5	1
1:C:684:ILE:HD12	1:C:684:ILE:N	0.41	2.31	14	1
1:A:755:LEU:HD22	1:A:755:LEU:C	0.41	2.40	15	1
1:B:774:LEU:HD21	1:C:742:ARG:CZ	0.40	2.47	2	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.40	2.30	4	1
1:B:758:ASP:OD1	1:C:715:LEU:HD22	0.40	2.15	4	1
1:A:765:LEU:HD23	1:A:765:LEU:C	0.40	2.42	5	1
1:B:677:ASN:OD1	1:B:681:TYR:CZ	0.40	2.74	6	1
1:C:774:LEU:HD13	1:C:777:ILE:HD12	0.40	1.93	7	1
1:A:763:LEU:O	1:A:774:LEU:HD23	0.40	2.16	8	1
1:B:704:LEU:HD11	1:C:712:TYR:O	0.40	2.16	12	1
1:B:747:ARG:C	1:B:747:ARG:HD3	0.40	2.41	12	1
1:A:777:ILE:O	1:A:781:ILE:HD13	0.40	2.15	8	1
1:B:745:SER:O	1:B:748:LEU:HD12	0.40	2.16	5	1
1:B:708:VAL:HG11	1:B:748:LEU:HD12	0.40	1.93	1	1
1:A:771:LEU:C	1:A:771:LEU:HD23	0.40	2.40	2	1
1:B:679:LEU:O	1:B:682:ILE:HD12	0.40	2.16	10	1
1:C:679:LEU:O	1:C:679:LEU:HD13	0.40	2.17	12	1
1:B:775:LEU:O	1:B:778:VAL:HG22	0.40	2.17	14	1
1:C:770:ARG:O	1:C:773:ASP:CG	0.40	2.64	14	1
1:A:663:LEU:HD23	1:A:663:LEU:C	0.40	2.42	1	1
1:C:705:VAL:HG13	1:C:748:LEU:CD1	0.40	2.47	2	1
1:A:675:ILE:CD1	1:A:679:LEU:HD23	0.40	2.46	4	1
1:B:660:LEU:O	1:B:661:LEU:HD22	0.40	2.16	4	1
1:C:660:LEU:HD12	1:C:660:LEU:O	0.40	2.16	9	1
1:A:663:LEU:HD23	1:A:664:ASP:N	0.40	2.32	14	1
1:A:781:ILE:HG13	1:B:746:ILE:HG21	0.40	1.92	15	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	101/129 (78%)	93±1 (92±1%)	6±1 (5±1%)	2±1 (2±1%)	7	45
1	B	103/129 (80%)	95±2 (92±2%)	5±2 (5±2%)	3±1 (3±1%)	6	40
1	C	99/129 (77%)	92±1 (93±1%)	4±1 (4±1%)	3±1 (3±1%)	5	38
All	All	4545/5805 (78%)	4207 (93%)	215 (5%)	123 (3%)	6	41

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	661	LEU	14
1	C	714	PRO	13
1	A	661	LEU	11
1	A	714	PRO	11
1	B	714	PRO	11
1	B	766	PHE	8
1	C	661	LEU	8
1	C	766	PHE	8
1	A	765	LEU	7
1	C	768	TYR	4
1	C	767	SER	4
1	C	765	LEU	4
1	A	712	TYR	3
1	B	765	LEU	3
1	B	662	GLU	3
1	B	767	SER	2
1	C	674	ASP	2
1	B	673	PHE	1
1	B	674	ASP	1
1	A	767	SER	1
1	A	768	TYR	1
1	C	673	PHE	1
1	C	769	HIS	1
1	A	674	ASP	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	97/117 (83%)	74±3 (77±3%)	23±3 (23±3%)	2	27
1	B	99/117 (85%)	76±3 (77±3%)	23±3 (23±3%)	2	28
1	C	95/117 (81%)	76±3 (80±3%)	19±3 (20±3%)	3	32
All	All	4365/5265 (83%)	3389 (78%)	976 (22%)	2	29

All 222 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	692	LEU	15
1	B	693	ILE	15
1	B	701	VAL	15
1	C	704	LEU	15
1	A	704	LEU	14
1	B	692	LEU	14
1	B	704	LEU	14
1	A	708	VAL	13
1	C	708	VAL	13
1	C	675	ILE	13
1	A	693	ILE	12
1	A	785	LEU	12
1	A	749	VAL	11
1	B	695	LEU	11
1	B	697	ILE	11
1	C	663	LEU	11
1	C	701	VAL	11
1	A	679	LEU	11
1	B	780	ARG	11
1	C	780	ARG	11
1	A	763	LEU	10
1	B	679	LEU	10
1	B	685	PHE	10
1	B	708	VAL	10
1	A	715	LEU	10
1	B	763	LEU	10
1	B	774	LEU	10
1	A	695	LEU	9
1	A	744	ARG	9
1	A	746	ILE	9
1	B	775	LEU	9
1	C	660	LEU	9
1	C	746	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	662	GLU	9
1	B	741	ASP	9
1	B	768	TYR	9
1	C	662	GLU	9
1	A	660	LEU	8
1	A	747	ARG	8
1	B	747	ARG	8
1	B	787	ARG	8
1	C	679	LEU	8
1	C	693	ILE	8
1	C	692	LEU	8
1	C	772	ARG	8
1	B	660	LEU	8
1	A	698	VAL	7
1	A	748	LEU	7
1	B	662	GLU	7
1	C	748	LEU	7
1	C	774	LEU	7
1	A	780	ARG	7
1	A	764	SER	7
1	C	665	LYS	7
1	B	765	LEU	7
1	A	682	ILE	7
1	B	746	ILE	7
1	A	710	GLN	6
1	A	712	TYR	6
1	C	688	ILE	6
1	A	663	LEU	6
1	C	763	LEU	6
1	A	741	ASP	6
1	A	750	ASN	6
1	A	771	LEU	5
1	B	713	SER	5
1	C	710	GLN	5
1	C	739	GLU	5
1	B	663	LEU	5
1	B	760	LEU	5
1	C	760	LEU	5
1	A	664	ASP	5
1	B	748	LEU	5
1	C	685	PHE	5
1	C	764	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	C	776	LEU	5
1	C	668	SER	5
1	C	678	TRP	5
1	A	765	LEU	5
1	B	742	ARG	5
1	A	683	ARG	4
1	B	744	ARG	4
1	B	766	PHE	4
1	C	768	TYR	4
1	B	772	ARG	4
1	A	661	LEU	4
1	A	685	PHE	4
1	A	774	LEU	4
1	B	739	GLU	4
1	B	785	LEU	4
1	B	661	LEU	4
1	C	744	ARG	4
1	C	765	LEU	4
1	C	674	ASP	4
1	A	702	LEU	4
1	B	698	VAL	4
1	A	775	LEU	3
1	A	777	ILE	3
1	B	769	HIS	3
1	B	779	THR	3
1	C	707	ARG	3
1	C	766	PHE	3
1	C	775	LEU	3
1	A	740	ARG	3
1	A	742	ARG	3
1	C	680	TRP	3
1	C	747	ARG	3
1	B	665	LYS	3
1	B	686	ILE	3
1	B	743	ASP	3
1	B	770	ARG	3
1	C	715	LEU	3
1	B	671	ASN	3
1	B	706	ASN	3
1	A	688	ILE	3
1	A	768	TYR	3
1	B	682	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	669	LEU	3
1	A	675	ILE	3
1	C	691	SER	3
1	C	745	SER	3
1	B	675	ILE	3
1	B	707	ARG	3
1	B	764	SER	3
1	A	755	LEU	3
1	A	776	LEU	2
1	B	778	VAL	2
1	C	697	ILE	2
1	A	674	ASP	2
1	B	674	ASP	2
1	B	745	SER	2
1	B	755	LEU	2
1	C	661	LEU	2
1	A	779	THR	2
1	B	683	ARG	2
1	B	710	GLN	2
1	A	665	LYS	2
1	A	671	ASN	2
1	A	760	LEU	2
1	C	695	LEU	2
1	C	783	GLU	2
1	A	696	ARG	2
1	A	709	ARG	2
1	A	762	SER	2
1	A	784	LEU	2
1	B	696	ARG	2
1	C	749	VAL	2
1	B	761	ARG	2
1	C	759	ASP	2
1	A	739	GLU	2
1	C	741	ASP	2
1	C	767	SER	2
1	C	781	ILE	2
1	A	705	VAL	2
1	A	781	ILE	2
1	B	776	LEU	2
1	B	777	ILE	2
1	C	706	ASN	2
1	C	713	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	C	777	ILE	2
1	A	678	TRP	2
1	A	697	ILE	2
1	A	699	PHE	2
1	B	762	SER	2
1	C	709	ARG	2
1	A	716	SER	2
1	A	767	SER	2
1	C	779	THR	2
1	A	772	ARG	2
1	B	740	ARG	1
1	B	784	LEU	1
1	A	668	SER	1
1	A	714	PRO	1
1	C	740	ARG	1
1	C	773	ASP	1
1	A	745	SER	1
1	B	703	SER	1
1	B	668	SER	1
1	B	716	SER	1
1	B	771	LEU	1
1	A	713	SER	1
1	A	770	ARG	1
1	B	752	SER	1
1	C	669	LEU	1
1	C	676	THR	1
1	C	770	ARG	1
1	A	758	ASP	1
1	B	709	ARG	1
1	B	788	ARG	1
1	A	676	THR	1
1	A	701	VAL	1
1	B	664	ASP	1
1	B	691	SER	1
1	B	749	VAL	1
1	B	757	TRP	1
1	A	686	ILE	1
1	A	707	ARG	1
1	A	783	GLU	1
1	B	673	PHE	1
1	C	742	ARG	1
1	C	750	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	C	761	ARG	1
1	B	773	ASP	1
1	C	771	LEU	1
1	B	712	TYR	1
1	B	781	ILE	1
1	B	783	GLU	1
1	C	673	PHE	1
1	C	705	VAL	1
1	A	703	SER	1
1	B	678	TRP	1
1	B	715	LEU	1
1	A	743	ASP	1
1	A	773	ASP	1
1	C	683	ARG	1
1	C	716	SER	1
1	B	759	ASP	1
1	C	703	SER	1
1	A	769	HIS	1
1	A	706	ASN	1
1	C	762	SER	1
1	C	769	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *HIV1_gp41_MPER-TMD-CTLLP2_chemical_shifts.tab*

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	520
Number of shifts mapped to atoms	427
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 93 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	717	PHE	H	8.06	0.01	1
1	A	717	PHE	C	175.39	0.05	1
1	A	717	PHE	CA	57.46	0.05	1
1	A	717	PHE	CB	38.33	0.05	1
1	A	717	PHE	N	120.76	0.03	1
1	A	718	GLN	H	8.15	0.01	1
1	A	718	GLN	C	175.83	0.05	1
1	A	718	GLN	CA	55.52	0.05	1
1	A	718	GLN	CB	28.72	0.05	1
1	A	718	GLN	N	119.94	0.03	1
1	A	719	THR	H	8.04	0.01	1
1	A	719	THR	CA	61.73	0.05	1
1	A	719	THR	CB	68.95	0.05	1
1	A	719	THR	N	113.98	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	720	HIS	C	174.61	0.05	1
1	A	720	HIS	CA	55.59	0.05	1
1	A	720	HIS	CB	29.94	0.05	1
1	A	721	LEU	H	8.03	0.01	1
1	A	721	LEU	CA	52.32	0.05	1
1	A	721	LEU	CB	40.6	0.05	1
1	A	721	LEU	N	123.72	0.03	1
1	A	722	PRO	C	176.55	0.05	1
1	A	722	PRO	CA	62.43	0.05	1
1	A	722	PRO	CB	30.9	0.05	1
1	A	723	THR	H	8.17	0.01	1
1	A	723	THR	CA	59.3	0.05	1
1	A	723	THR	CB	68.95	0.05	1
1	A	723	THR	N	116.44	0.03	1
1	A	724	PRO	C	176.7	0.05	1
1	A	724	PRO	CA	62.79	0.05	1
1	A	724	PRO	CB	31.23	0.05	1
1	A	725	ARG	H	8.37	0.01	1
1	A	725	ARG	C	176.44	0.05	1
1	A	725	ARG	CA	55.51	0.05	1
1	A	725	ARG	CB	30.18	0.05	1
1	A	725	ARG	N	121.04	0.03	1
1	A	726	GLY	H	8.23	0.01	1
1	A	726	GLY	C	171.92	0.05	1
1	A	726	GLY	CA	44.04	0.05	1
1	A	726	GLY	N	110.02	0.03	1
1	A	727	PRO	C	176.72	0.05	1
1	A	727	PRO	CA	62.84	0.05	1
1	A	727	PRO	CB	31.14	0.05	1
1	A	728	ASP	H	8.38	0.01	1
1	A	728	ASP	C	175.65	0.05	1
1	A	728	ASP	CA	54.07	0.05	1
1	A	728	ASP	CB	40.05	0.05	1
1	A	728	ASP	N	119.29	0.03	1
1	A	729	ARG	H	8.02	0.01	1
1	A	729	ARG	C	174.0	0.05	1
1	A	729	ARG	CA	53.08	0.05	1
1	A	729	ARG	CB	29.34	0.05	1
1	A	729	ARG	N	120.86	0.03	1
1	A	730	PRO	C	176.84	0.05	1
1	A	730	PRO	CA	62.79	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	730	PRO	CB	31.09	0.05	1
1	A	731	GLU	H	8.57	0.01	1
1	A	731	GLU	C	177.03	0.05	1
1	A	731	GLU	CA	56.43	0.05	1
1	A	731	GLU	CB	29.29	0.05	1
1	A	731	GLU	N	120.32	0.03	1
1	A	732	GLY	H	8.36	0.01	1
1	A	732	GLY	C	173.94	0.05	1
1	A	732	GLY	CA	44.91	0.05	1
1	A	732	GLY	N	109.52	0.03	1
1	A	733	ILE	H	7.82	0.01	1
1	A	733	ILE	C	176.16	0.05	1
1	A	733	ILE	CA	60.51	0.05	1
1	A	733	ILE	CB	37.61	0.05	1
1	A	733	ILE	N	119.17	0.03	1
1	A	734	GLU	H	8.49	0.01	1
1	A	734	GLU	C	176.36	0.05	1
1	A	734	GLU	CA	56.11	0.05	1
1	A	734	GLU	CB	29.31	0.05	1
1	A	734	GLU	N	124.32	0.03	1
1	A	735	GLU	H	8.38	0.01	1
1	A	735	GLU	C	176.48	0.05	1
1	A	735	GLU	CA	56.11	0.05	1
1	A	735	GLU	CB	29.46	0.05	1
1	A	735	GLU	N	121.83	0.03	1
1	A	736	GLU	H	8.47	0.01	1
1	A	736	GLU	C	177.09	0.05	1
1	A	736	GLU	CA	56.32	0.05	1
1	A	736	GLU	CB	29.38	0.05	1
1	A	736	GLU	N	122.08	0.03	1
1	A	737	GLY	H	8.51	0.01	1
1	A	737	GLY	C	174.82	0.05	1
1	A	737	GLY	CA	45.04	0.05	1
1	A	737	GLY	N	109.96	0.03	1
1	A	738	GLY	H	8.27	0.01	1
1	A	738	GLY	C	174.5	0.05	1
1	A	738	GLY	CA	44.95	0.05	1
1	A	738	GLY	N	108.53	0.03	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	120	0.00 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	55	1.26 ± 0.13	Should be checked
$^{13}\text{C}'$	113	-0.13 ± 0.13	None needed (< 0.5 ppm)
^{15}N	116	0.72 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 9%, i.e. 414 atoms were assigned a chemical shift out of a possible 4852. 0 out of 88 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	379/1572 (24%)	96/636 (15%)	187/626 (30%)	96/310 (31%)
Sidechain	35/2839 (1%)	0/1867 (0%)	35/840 (4%)	0/132 (0%)
Aromatic	0/441 (0%)	0/216 (0%)	0/201 (0%)	0/24 (0%)
Overall	414/4852 (9%)	96/2719 (4%)	222/1667 (13%)	96/466 (21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 427 atoms were assigned a chemical shift out of a possible 4992. 0 out of 90 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	390/1614 (24%)	99/654 (15%)	192/642 (30%)	99/318 (31%)
Sidechain	37/2937 (1%)	0/1929 (0%)	37/864 (4%)	0/144 (0%)
Aromatic	0/441 (0%)	0/216 (0%)	0/201 (0%)	0/24 (0%)
Overall	427/4992 (9%)	99/2799 (4%)	229/1707 (13%)	99/486 (20%)

7.1.4 Statistically unusual chemical shifts ⓘ

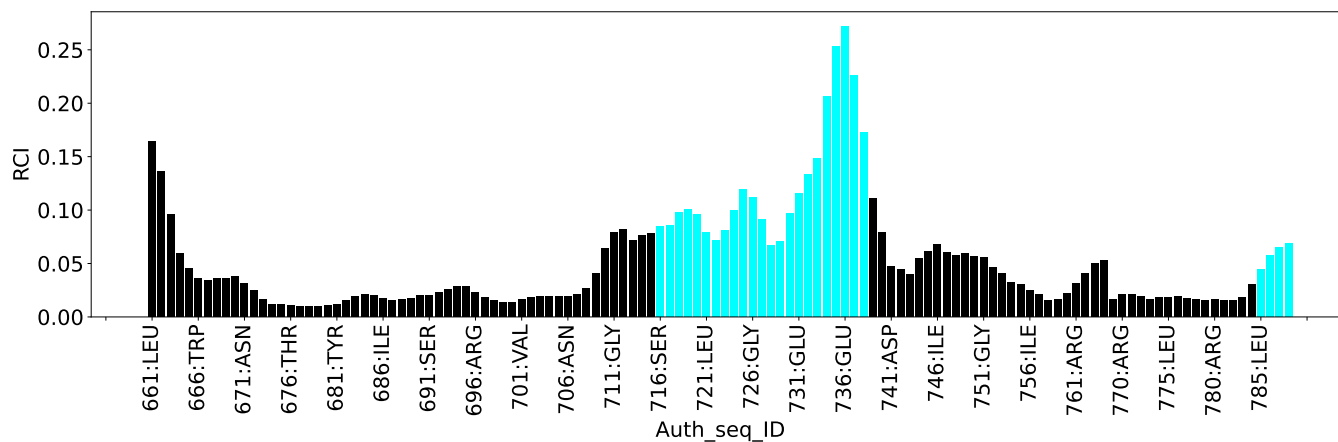
There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1425
Intra-residue ($ i-j =0$)	192
Sequential ($ i-j =1$)	498
Medium range ($ i-j >1$ and $ i-j <5$)	525
Long range ($ i-j \geq 5$)	117
Inter-chain	0
Hydrogen bond restraints	93
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	38
Number of restraints per residue	4.1
Number of long range restraints per residue ¹	0.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	75.2	0.2
0.2-0.5 (Medium)	88.0	0.5
>0.5 (Large)	135.6	29.07

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	17.4	4.34
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

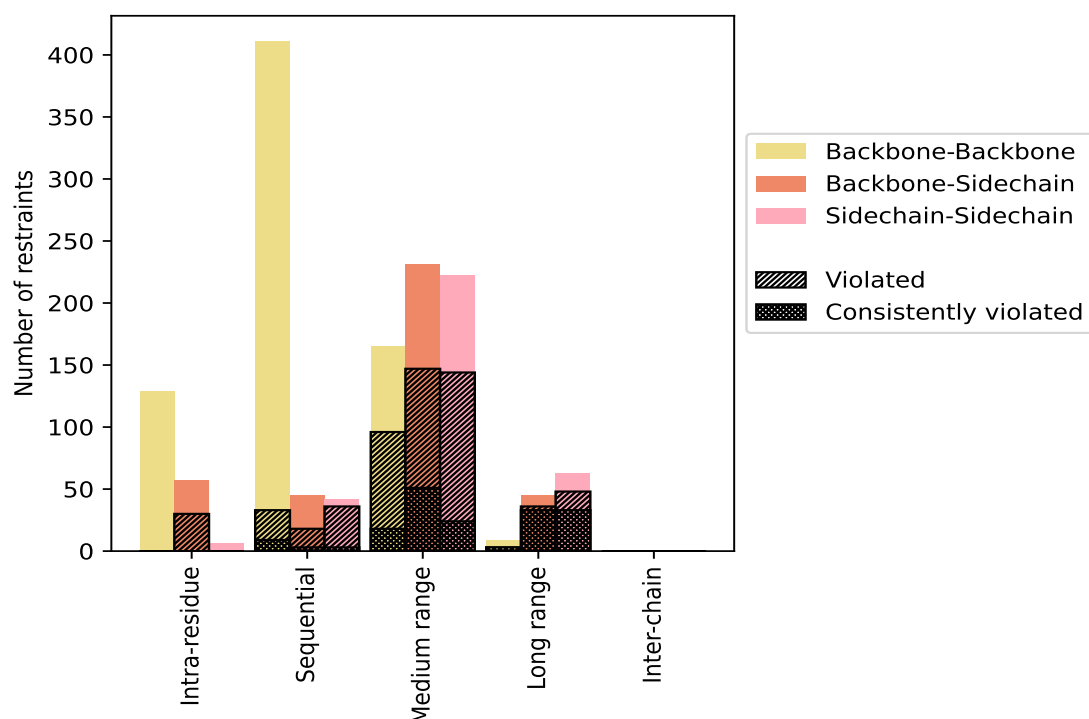
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	192	13.5	30	15.6	2.1	0	0.0	0.0
Backbone-Backbone	129	9.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	4.0	30	52.6	2.1	0	0.0	0.0
Sidechain-Sidechain	6	0.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	498	34.9	87	17.5	6.1	15	3.0	1.1
Backbone-Backbone	411	28.8	33	8.0	2.3	9	2.2	0.6
Backbone-Sidechain	45	3.2	18	40.0	1.3	3	6.7	0.2
Sidechain-Sidechain	42	2.9	36	85.7	2.5	3	7.1	0.2
Medium range ($i-j >1$ & $i-j <5$)	525	36.8	315	60.0	22.1	60	11.4	4.2
Backbone-Backbone	165	11.6	96	58.2	6.7	18	10.9	1.3
Backbone-Sidechain	153	10.7	90	58.8	6.3	18	11.8	1.3
Sidechain-Sidechain	207	14.5	129	62.3	9.1	24	11.6	1.7
Long range ($i-j \geq 5$)	117	8.2	87	74.4	6.1	69	59.0	4.8
Backbone-Backbone	9	0.6	3	33.3	0.2	3	33.3	0.2
Backbone-Sidechain	45	3.2	36	80.0	2.5	33	73.3	2.3
Sidechain-Sidechain	63	4.4	48	76.2	3.4	33	52.4	2.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	93	6.5	72	77.4	5.1	33	35.5	2.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1425	100.0	591	41.5	41.5	177	12.4	12.4
Backbone-Backbone	714	50.1	132	18.5	9.3	30	4.2	2.1
Backbone-Sidechain	378	26.5	231	61.1	16.2	87	23.0	6.1
Sidechain-Sidechain	333	23.4	228	68.5	16.0	60	18.0	4.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	6	27	165	72	0	270	4.18	27.75	7.68	0.48
2	15	30	183	75	0	303	3.77	28.91	7.51	0.37
3	15	30	177	75	0	297	3.9	28.36	7.42	0.45
4	12	30	174	78	0	294	3.88	28.66	7.45	0.42
5	12	30	177	75	0	294	3.9	27.57	7.42	0.39
6	15	30	189	75	0	309	3.74	28.52	7.28	0.42
7	9	33	186	72	0	300	3.85	29.07	7.55	0.42
8	9	54	195	72	0	330	3.52	27.54	7.12	0.38
9	6	36	195	81	0	318	3.56	28.3	7.18	0.32
10	12	30	183	69	0	294	3.99	28.9	7.64	0.49

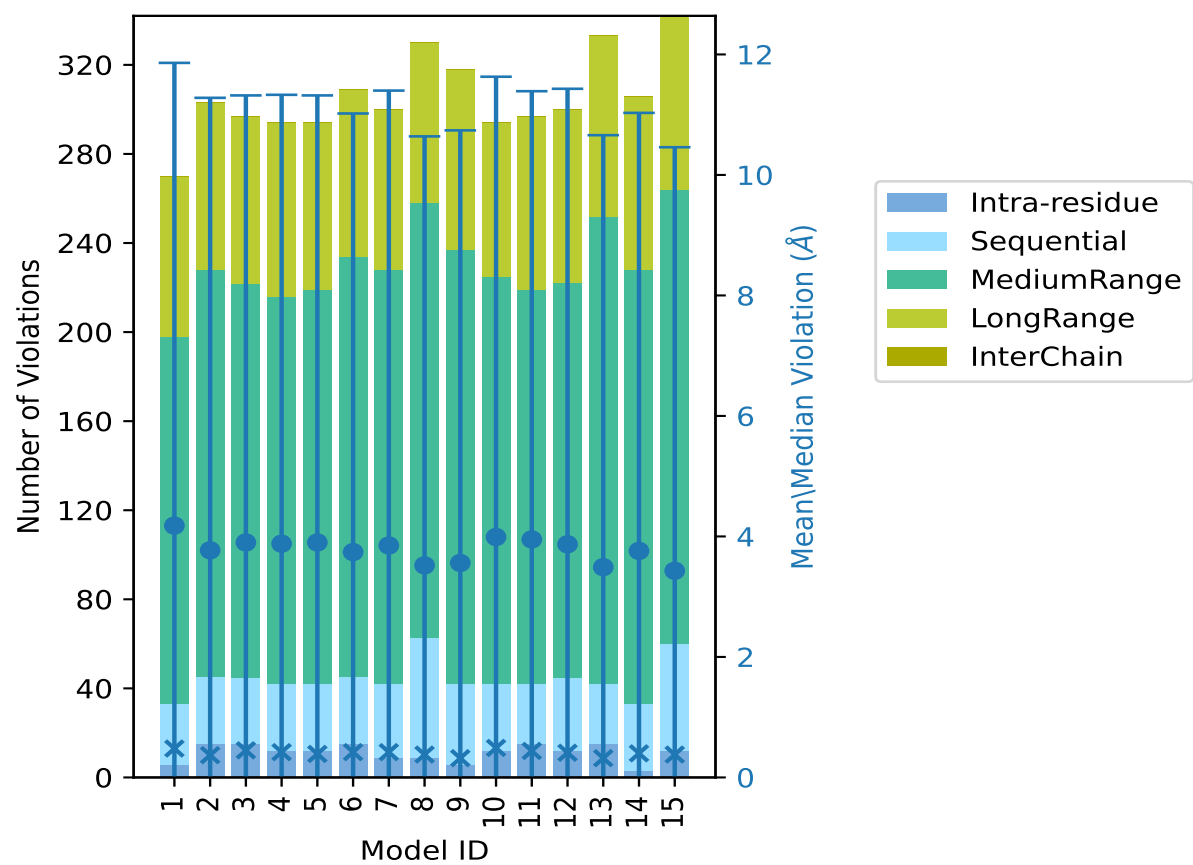
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	15	27	177	78	0	297	3.95	27.96	7.44	0.44
12	12	33	177	78	0	300	3.87	29.03	7.56	0.41
13	15	27	210	81	0	333	3.49	28.75	7.17	0.32
14	3	30	195	78	0	306	3.76	28.1	7.27	0.4
15	12	48	204	78	0	342	3.43	28.09	7.03	0.38

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

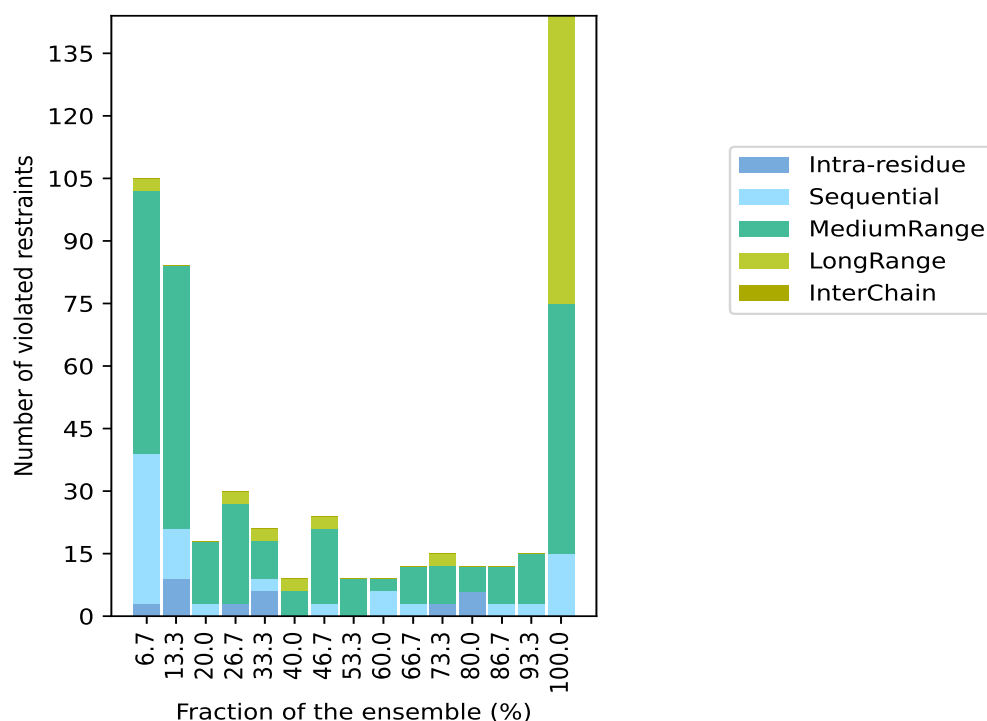
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 813(IR:162, SQ:411, MR:210, LR:30, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	36	63	3	0	105	1	6.7
9	12	63	0	0	84	2	13.3
0	3	15	0	0	18	3	20.0
3	0	24	3	0	30	4	26.7
6	3	9	3	0	21	5	33.3
0	0	6	3	0	9	6	40.0
0	3	18	3	0	24	7	46.7
0	0	9	0	0	9	8	53.3
0	6	3	0	0	9	9	60.0
0	3	9	0	0	12	10	66.7
3	0	9	3	0	15	11	73.3
6	0	6	0	0	12	12	80.0
0	3	9	0	0	12	13	86.7
0	3	12	0	0	15	14	93.3
0	15	60	69	0	144	15	100.0

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

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

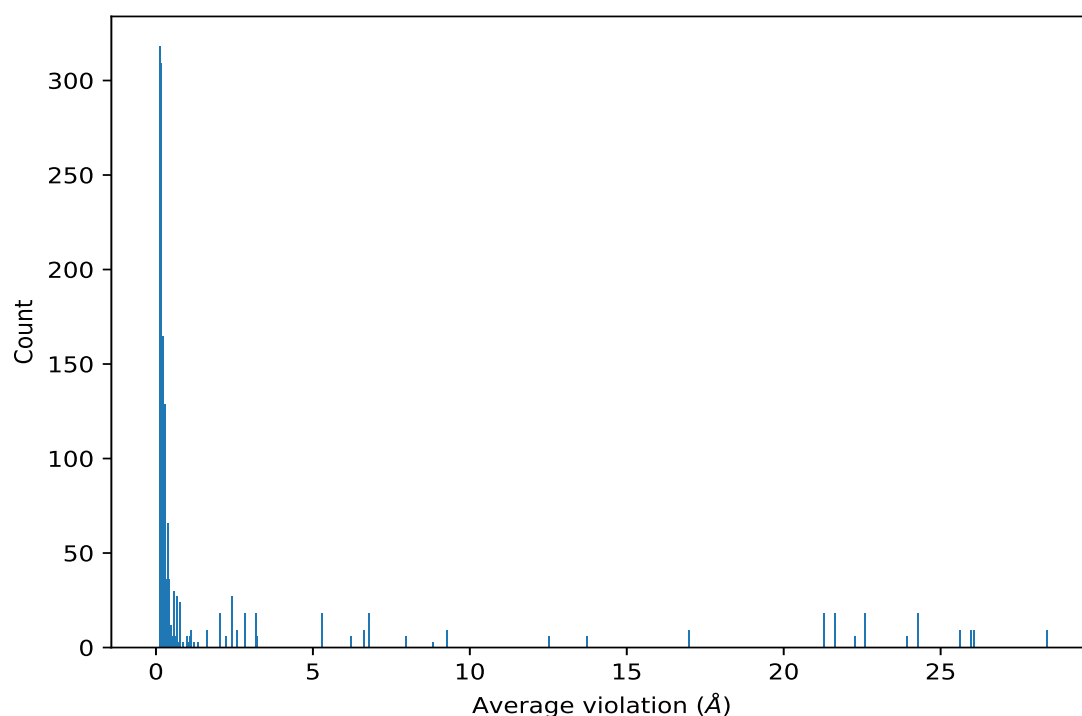
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.37	0.5	28.36
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.37	0.5	28.36
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.37	0.5	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.37	0.5	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.37	0.5	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.37	0.5	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.37	0.5	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.37	0.5	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.37	0.5	28.36
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	26.05	0.59	25.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	26.05	0.59	25.96
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.97	0.69	25.75
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.6	0.62	25.44
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.28	0.47	24.38
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.28	0.47	24.38
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.94	0.53	23.91
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.94	0.53	23.91
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.94	0.53	23.91
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.94	0.53	23.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.94	0.53	23.91
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.94	0.53	23.91
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	22.57	0.73	22.55
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	22.57	0.73	22.55
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.29	0.47	22.28
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.29	0.47	22.28
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.29	0.47	22.28
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.29	0.47	22.28
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.29	0.47	22.28
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.29	0.47	22.28
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.62	1.26	22.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.62	1.26	22.0
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.62	1.26	22.0
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.29	0.34	21.19
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.29	0.34	21.19
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	16.99	0.53	16.8
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	16.99	0.53	16.8
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	16.99	0.53	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	16.99	0.53	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	16.99	0.53	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	16.99	0.53	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	16.99	0.53	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	16.99	0.53	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	16.99	0.53	16.8
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	13.74	0.31	13.7
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	13.74	0.31	13.7
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	13.74	0.31	13.7
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	13.74	0.31	13.7
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	13.74	0.31	13.7
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	13.74	0.31	13.7
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.53	0.5	12.54
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.53	0.5	12.54
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.53	0.5	12.54
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.53	0.5	12.54
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.53	0.5	12.54
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.53	0.5	12.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.25	0.33	9.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.25	0.33	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.25	0.33	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.25	0.33	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.25	0.33	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.25	0.33	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.25	0.33	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.25	0.33	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.25	0.33	9.24
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.8	0.34	8.85
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.8	0.34	8.85
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.8	0.34	8.85
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.97	0.49	7.82
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.97	0.49	7.82
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.97	0.49	7.82
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.97	0.49	7.82
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.97	0.49	7.82
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.97	0.49	7.82
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	6.76	1.03	6.77
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	6.76	1.03	6.77
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	6.64	0.38	6.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	6.64	0.38	6.68
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	6.2	0.65	6.36
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	6.2	0.65	6.36
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	6.2	0.65	6.36
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	6.2	0.65	6.36
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	6.2	0.65	6.36
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	6.2	0.65	6.36
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.27	0.41	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.27	0.41	5.32
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.24	0.61	3.3
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.24	0.61	3.3
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.24	0.61	3.3
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.24	0.61	3.3
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.24	0.61	3.3
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.24	0.61	3.3
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.16	0.42	3.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.16	0.42	3.08
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.81	0.8	2.53
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.81	0.8	2.53
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.55	0.4	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.55	0.4	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.55	0.4	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.55	0.4	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.55	0.4	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.55	0.4	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.55	0.4	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.55	0.4	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.55	0.4	2.61
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.42	0.06	2.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.42	0.06	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.42	0.06	2.42
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.21	0.27	2.26
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.21	0.27	2.26
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.21	0.27	2.26
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.21	0.27	2.26
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.21	0.27	2.26
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.21	0.27	2.26
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.02	0.15	2.07

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.02	0.15	2.07
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.02	0.15	2.07
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.6	0.18	1.65
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.6	0.18	1.65
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	15	1.33	0.22	1.37
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	15	1.33	0.22	1.37
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	15	1.33	0.22	1.37
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.23	0.12	1.26
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.23	0.12	1.26
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.23	0.12	1.26
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.1	0.18	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.1	0.18	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.1	0.18	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.1	0.18	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.1	0.18	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.1	0.18	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.1	0.18	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.1	0.18	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.1	0.18	1.15
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	15	1.08	0.2	1.07
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	15	1.08	0.2	1.07
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	15	1.08	0.2	1.07
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.07	0.11	1.08
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.07	0.11	1.08
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.07	0.11	1.08
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	15	1.01	0.22	1.05
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	15	1.01	0.22	1.05
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	15	1.01	0.22	1.05
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.87	0.29	0.81
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.87	0.29	0.81
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.87	0.29	0.81
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.77	0.21	0.79
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.77	0.21	0.79
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.77	0.21	0.79
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.77	0.39	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.77	0.39	0.62
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.77	0.39	0.62
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	15	0.67	0.26	0.66
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	15	0.67	0.26	0.66
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.67	0.18	0.71
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.67	0.18	0.71
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.67	0.18	0.71
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.6	0.19	0.61
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.6	0.19	0.61
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.6	0.19	0.61
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.57	0.25	0.47
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.57	0.25	0.47
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.57	0.25	0.47
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.55	0.09	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.55	0.09	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.55	0.09	0.55
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.53	0.12	0.58
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.53	0.12	0.58
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.53	0.12	0.58
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.53	0.12	0.58
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.53	0.12	0.58
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.53	0.12	0.58
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.44	0.14	0.49
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.38	0.09	0.38
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.38	0.09	0.38
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.38	0.09	0.38
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.37	0.12	0.37
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.37	0.12	0.37
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.37	0.12	0.37
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.37	0.09	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.37	0.09	0.34
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.37	0.09	0.34
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.35	0.09	0.38
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33	0.07	0.32
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33	0.07	0.32
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33	0.07	0.32
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.32	0.05	0.33
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.32	0.05	0.33
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.32	0.05	0.33
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.28	0.07	0.25
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.28	0.07	0.25
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.28	0.07	0.25
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.26	0.08	0.28
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.26	0.07	0.26
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.26	0.07	0.26
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.26	0.07	0.26
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.25	0.05	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.25	0.05	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.25	0.05	0.27
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.23	0.1	0.2
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.23	0.1	0.2
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22	0.04	0.22
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22	0.04	0.22
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22	0.04	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.21	0.01	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.21	0.01	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.21	0.01	0.21
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21	0.01	0.21
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21	0.01	0.21
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21	0.01	0.21
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18	0.01	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18	0.01	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18	0.01	0.18
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.78	0.42	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.78	0.42	0.68
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.78	0.42	0.68
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.71	0.36	0.6
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.71	0.36	0.6
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.71	0.36	0.6
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.45	0.14	0.52
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.45	0.14	0.52
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.45	0.14	0.52
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.45	0.14	0.52
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.45	0.14	0.52
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.45	0.14	0.52
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.25	0.05	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.25	0.05	0.27
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.24	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.24	0.04	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.24	0.04	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.24	0.04	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.24	0.04	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.24	0.04	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.24	0.04	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.24	0.04	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.24	0.04	0.25
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.23	0.05	0.23
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.23	0.05	0.23
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.23	0.05	0.23
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.31	0.05	0.29
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.31	0.1	0.28
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.31	0.1	0.28
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.31	0.1	0.28
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17	0.08	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17	0.08	0.13
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.15	0.04	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.15	0.04	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.15	0.04	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.15	0.04	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.15	0.04	0.14
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.43	0.19	0.44
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,535)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.43	0.19	0.44
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,941)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.43	0.19	0.44
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,1347)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	12	0.43	0.19	0.44
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.36	0.13	0.34
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.36	0.13	0.34
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.36	0.13	0.34
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.36	0.13	0.34
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.36	0.13	0.34
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.36	0.13	0.34
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.32	0.16	0.31
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.32	0.16	0.31
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.32	0.16	0.31
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.27	0.12	0.26
(2,533)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.27	0.12	0.26
(2,939)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.27	0.12	0.26
(2,1345)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	12	0.27	0.12	0.26
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	12	0.23	0.12	0.2
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	12	0.23	0.12	0.2
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	12	0.23	0.12	0.2
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	12	0.23	0.12	0.2
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	12	0.23	0.12	0.2
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	12	0.23	0.12	0.2
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	12	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	12	0.16	0.02	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	12	0.16	0.02	0.16
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.45	0.13	0.52
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.45	0.13	0.52
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.45	0.13	0.52
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	11	0.27	0.13	0.24
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	11	0.27	0.13	0.24
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	11	0.27	0.13	0.24
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19	0.06	0.19
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19	0.06	0.19
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19	0.06	0.19
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	11	0.16	0.03	0.15
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	11	0.16	0.03	0.15
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	11	0.16	0.03	0.15
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.15	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.15	0.04	0.16
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.15	0.04	0.16
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.27	0.13	0.34
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.27	0.13	0.34
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.19	0.1	0.16
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.19	0.1	0.16
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.19	0.1	0.16
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16	0.03	0.18
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16	0.03	0.18
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16	0.03	0.18
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.16	0.03	0.16
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.16	0.03	0.16
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.16	0.03	0.16
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.44	0.15	0.52
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.18	0.09	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.18	0.09	0.16
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.18	0.09	0.16
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.13	0.02	0.14
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	8	0.35	0.16	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,532)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,532)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,532)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,532)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,938)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	8	0.35	0.16	0.3
(2,1344)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	8	0.35	0.16	0.3
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	8	0.3	0.18	0.22
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	8	0.3	0.18	0.22
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	8	0.3	0.18	0.22
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	8	0.3	0.18	0.22
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	8	0.3	0.18	0.22
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	8	0.3	0.18	0.22
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.22	0.14	0.18
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.22	0.14	0.18
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.22	0.14	0.18
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	8	0.19	0.07	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	8	0.19	0.07	0.18
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	8	0.19	0.07	0.18
(2,534)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.36	0.21	0.29
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,534)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,940)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.36	0.21	0.29
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,940)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,1346)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.36	0.21	0.29
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,1346)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	7	0.36	0.21	0.29
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25	0.08	0.25
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25	0.08	0.25
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.23	0.14	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.23	0.14	0.12
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.23	0.14	0.12
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.2	0.11	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.2	0.11	0.16
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	7	0.19	0.08	0.18
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	7	0.19	0.08	0.18
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	7	0.19	0.08	0.18
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15	0.03	0.15
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	7	0.13	0.02	0.12
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	7	0.13	0.02	0.12
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	7	0.13	0.02	0.12
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.13	0.03	0.13
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.13	0.03	0.13
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.13	0.03	0.13
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.13	0.02	0.13
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.13	0.02	0.13
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.13	0.02	0.13
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.31	0.14	0.31
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.31	0.14	0.31
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.31	0.14	0.31
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.31	0.14	0.31
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.31	0.14	0.31
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.31	0.14	0.31
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.31	0.14	0.31
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.31	0.14	0.31
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.31	0.14	0.31
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.22	0.08	0.21
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.22	0.08	0.21
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.22	0.08	0.21
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.22	0.08	0.21
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.22	0.08	0.21
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.22	0.08	0.21
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.13	0.03	0.12
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.98	0.19	1.01
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.98	0.19	1.01
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.98	0.19	1.01
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.98	0.19	1.01

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.98	0.19	1.01
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.98	0.19	1.01
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	5	0.46	0.05	0.46
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	5	0.46	0.05	0.46
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	5	0.46	0.05	0.46
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	5	0.21	0.04	0.21
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	5	0.18	0.04	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	5	0.18	0.04	0.18
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	5	0.17	0.03	0.16
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	5	0.14	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	5	0.14	0.04	0.13
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	5	0.14	0.04	0.13
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.12	0.02	0.11
(2,531)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,531)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	4	0.26	0.14	0.26
(2,531)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,937)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,937)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	4	0.26	0.14	0.26
(2,937)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,1343)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,1343)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	4	0.26	0.14	0.26
(2,1343)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	4	0.26	0.14	0.26
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	4	0.2	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	4	0.2	0.05	0.18
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	4	0.2	0.05	0.18
(2,422)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,422)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,422)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,828)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,828)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,828)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,1234)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,1234)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,1234)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	4	0.17	0.03	0.16
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB2	4	0.16	0.03	0.16
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB3	4	0.16	0.03	0.16
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB2	4	0.16	0.03	0.16
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB3	4	0.16	0.03	0.16
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB2	4	0.16	0.03	0.16
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB3	4	0.16	0.03	0.16
(2,338)	1:708:A:VAL:H	1:705:A:VAL:HA	4	0.15	0.03	0.16
(2,744)	1:708:A:VAL:H	1:705:A:VAL:HA	4	0.15	0.03	0.16
(2,1150)	1:708:A:VAL:H	1:705:A:VAL:HA	4	0.15	0.03	0.16
(2,353)	1:709:A:ARG:HE	1:709:A:ARG:H	4	0.14	0.06	0.11
(2,759)	1:709:A:ARG:HE	1:709:A:ARG:H	4	0.14	0.06	0.11
(2,1165)	1:709:A:ARG:HE	1:709:A:ARG:H	4	0.14	0.06	0.11
(2,150)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.13	0.03	0.12
(2,556)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.13	0.03	0.12
(2,962)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.13	0.03	0.12
(2,196)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,196)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,196)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,602)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,602)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,602)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,1008)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1008)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,1008)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.13	0.02	0.12
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.13	0.02	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.13	0.02	0.13
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	4	0.12	0.02	0.12
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	4	0.12	0.02	0.12
(2,175)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12	0.0	0.12
(2,581)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12	0.0	0.12
(2,987)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12	0.0	0.12
(2,309)	1:704:A:LEU:HD11	1:707:A:ARG:HE	3	0.2	0.09	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,309)	1:704:A:LEU:HD12	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,309)	1:704:A:LEU:HD13	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,715)	1:704:A:LEU:HD11	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,715)	1:704:A:LEU:HD12	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,715)	1:704:A:LEU:HD13	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,1121)	1:704:A:LEU:HD11	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,1121)	1:704:A:LEU:HD12	1:707:A:ARG:HE	3	0.2	0.09	0.13
(2,1121)	1:704:A:LEU:HD13	1:707:A:ARG:HE	3	0.2	0.09	0.13
(1,17)	1:753:C:LEU:O	1:757:C:TRP:H	3	0.18	0.02	0.19
(1,43)	1:753:C:LEU:O	1:757:C:TRP:H	3	0.18	0.02	0.19
(1,69)	1:753:C:LEU:O	1:757:C:TRP:H	3	0.18	0.02	0.19
(1,23)	1:756:C:ILE:O	1:760:C:LEU:H	3	0.16	0.05	0.15
(1,49)	1:756:C:ILE:O	1:760:C:LEU:H	3	0.16	0.05	0.15
(1,75)	1:756:C:ILE:O	1:760:C:LEU:H	3	0.16	0.05	0.15
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.14	0.03	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.14	0.03	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.12	0.01	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.12	0.01	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.12	0.01	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.12	0.01	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.12	0.01	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.12	0.01	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.12	0.01	0.12
(2,282)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,282)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,282)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,688)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,688)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,688)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,1094)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,1094)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,1094)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.11	0.01	0.11
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.11	0.01	0.11
(2,311)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.11	0.0	0.11
(2,717)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.11	0.0	0.11
(2,1123)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.11	0.0	0.11
(2,360)	1:710:A:GLN:H	1:710:A:GLN:HB2	2	0.62	0.02	0.62
(2,766)	1:710:A:GLN:H	1:710:A:GLN:HB2	2	0.62	0.02	0.62
(2,1172)	1:710:A:GLN:H	1:710:A:GLN:HB2	2	0.62	0.02	0.62
(2,319)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,319)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,319)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,725)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,725)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,725)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,1131)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,1131)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,1131)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.42	0.01	0.42
(2,317)	1:705:A:VAL:HG11	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,317)	1:705:A:VAL:HG12	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,317)	1:705:A:VAL:HG13	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,723)	1:705:A:VAL:HG11	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,723)	1:705:A:VAL:HG12	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,723)	1:705:A:VAL:HG13	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,1129)	1:705:A:VAL:HG11	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,1129)	1:705:A:VAL:HG12	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,1129)	1:705:A:VAL:HG13	1:706:A:ASN:HA	2	0.38	0.02	0.38
(2,431)	1:759:A:ASP:H	1:759:A:ASP:HB3	2	0.35	0.22	0.35
(2,837)	1:759:A:ASP:H	1:759:A:ASP:HB3	2	0.35	0.22	0.35
(2,1243)	1:759:A:ASP:H	1:759:A:ASP:HB3	2	0.35	0.22	0.35
(2,511)	1:784:A:LEU:H	1:781:A:ILE:HA	2	0.28	0.05	0.28
(2,917)	1:784:A:LEU:H	1:781:A:ILE:HA	2	0.28	0.05	0.28
(2,1323)	1:784:A:LEU:H	1:781:A:ILE:HA	2	0.28	0.05	0.28
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	2	0.25	0.14	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	2	0.25	0.14	0.25
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	2	0.25	0.14	0.25
(2,504)	1:782:A:VAL:HG21	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,504)	1:782:A:VAL:HG22	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,504)	1:782:A:VAL:HG23	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,910)	1:782:A:VAL:HG21	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,910)	1:782:A:VAL:HG22	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,910)	1:782:A:VAL:HG23	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,1316)	1:782:A:VAL:HG21	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,1316)	1:782:A:VAL:HG22	1:779:A:THR:HA	2	0.24	0.0	0.24
(2,1316)	1:782:A:VAL:HG23	1:779:A:THR:HA	2	0.24	0.0	0.24
(1,15)	1:747:C:ARG:O	1:751:C:GLY:H	2	0.22	0.01	0.22
(1,41)	1:747:C:ARG:O	1:751:C:GLY:H	2	0.22	0.01	0.22
(1,67)	1:747:C:ARG:O	1:751:C:GLY:H	2	0.22	0.01	0.22
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD11	2	0.2	0.0	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD12	2	0.2	0.0	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD13	2	0.2	0.0	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD21	2	0.2	0.0	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD22	2	0.2	0.0	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD23	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD11	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD12	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD13	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD21	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD22	2	0.2	0.0	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD23	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD11	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD12	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD13	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD21	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD22	2	0.2	0.0	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD23	2	0.2	0.0	0.2
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	2	0.17	0.01	0.17
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	2	0.17	0.01	0.17
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	2	0.17	0.01	0.17
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	2	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	2	0.17	0.01	0.17
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	2	0.17	0.01	0.17
(1,3)	1:741:C:ASP:O	1:745:C:SER:H	2	0.16	0.03	0.16
(1,29)	1:741:C:ASP:O	1:745:C:SER:H	2	0.16	0.03	0.16
(1,55)	1:741:C:ASP:O	1:745:C:SER:H	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.16	0.0	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.16	0.0	0.16
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.16	0.0	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.16	0.0	0.16
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	2	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	2	0.16	0.03	0.16
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	2	0.16	0.03	0.16
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.16	0.05	0.16
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.16	0.05	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.16	0.0	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.16	0.0	0.16
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	2	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	2	0.15	0.01	0.15
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	2	0.15	0.01	0.15
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	2	0.15	0.05	0.15
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	2	0.15	0.05	0.15
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.15	0.04	0.15
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.15	0.04	0.15
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,526)	1:786:A:GLY:H	1:782:A:VAL:HA	2	0.14	0.02	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	2	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,932)	1:786:A:GLY:H	1:782:A:VAL:HA	2	0.14	0.02	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	2	0.14	0.0	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	2	0.14	0.0	0.14
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	2	0.14	0.03	0.14
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	2	0.14	0.03	0.14
(2,1338)	1:786:A:GLY:H	1:782:A:VAL:HA	2	0.14	0.02	0.14
(2,169)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.14	0.02	0.14
(2,289)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.14	0.02	0.14
(2,575)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.14	0.02	0.14
(2,695)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.14	0.02	0.14
(2,981)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.14	0.02	0.14
(2,1101)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.14	0.02	0.14
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.13	0.01	0.13
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.13	0.01	0.13
(2,188)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.12	0.02	0.12
(2,271)	1:698:A:VAL:HG11	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,271)	1:698:A:VAL:HG12	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,271)	1:698:A:VAL:HG13	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,594)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.12	0.02	0.12
(2,677)	1:698:A:VAL:HG11	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,677)	1:698:A:VAL:HG12	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,677)	1:698:A:VAL:HG13	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,1000)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.12	0.02	0.12
(2,1083)	1:698:A:VAL:HG11	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,1083)	1:698:A:VAL:HG12	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,1083)	1:698:A:VAL:HG13	1:695:A:LEU:HG	2	0.12	0.02	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,493)	1:781:A:ILE:H	1:778:A:VAL:HA	2	0.12	0.01	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,899)	1:781:A:ILE:H	1:778:A:VAL:HA	2	0.12	0.01	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.12	0.0	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.12	0.0	0.12
(2,1305)	1:781:A:ILE:H	1:778:A:VAL:HA	2	0.12	0.01	0.12
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.12	0.02	0.12

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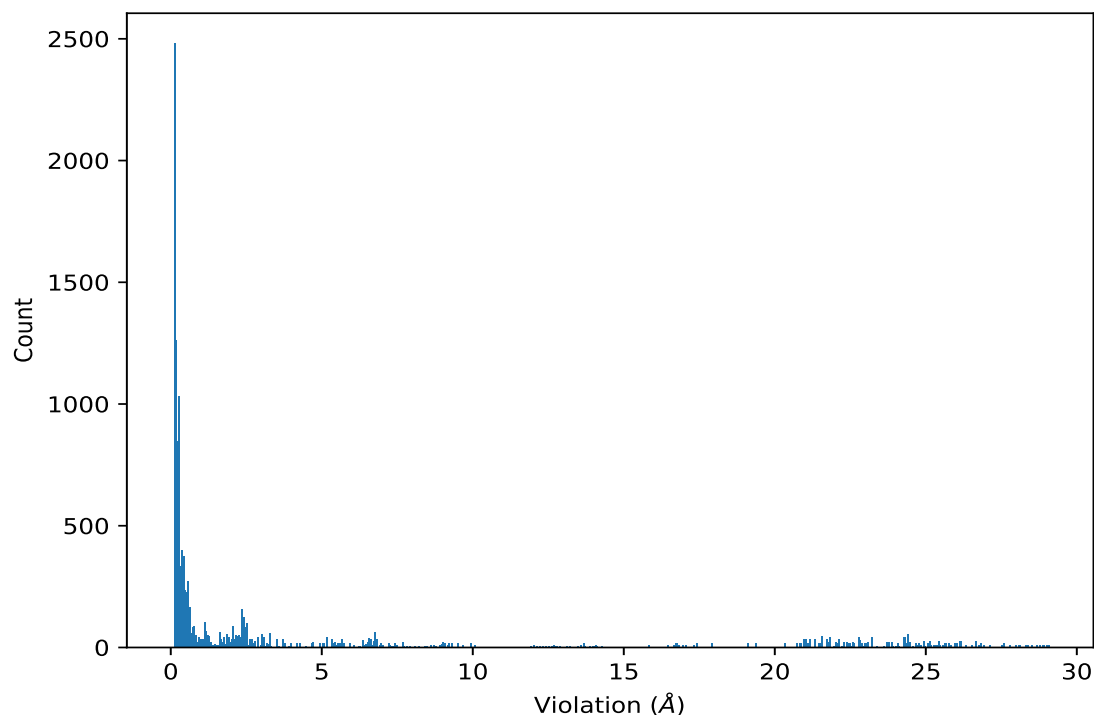
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(2,174)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,174)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,174)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,174)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,174)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,174)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,464)	1:776:A:LEU:H	1:773:A:ASP:HA	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,580)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,870)	1:776:A:LEU:H	1:773:A:ASP:HA	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,986)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.12	0.0	0.12
(2,1276)	1:776:A:LEU:H	1:773:A:ASP:HA	2	0.12	0.0	0.12

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)
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	7	29.07
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	7	29.07
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	7	29.07
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	7	29.07
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	7	29.07
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	7	29.07
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	7	29.07
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	7	29.07
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	7	29.07
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	12	29.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	12	29.03
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	12	29.03
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	12	29.03
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	12	29.03
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	12	29.03
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	12	29.03
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	12	29.03
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	12	29.03
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	2	28.91
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	2	28.91
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	2	28.91
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	2	28.91
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	2	28.91
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	2	28.91
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	2	28.91
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	2	28.91
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	2	28.91
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	10	28.9
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	10	28.9
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	10	28.9
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	10	28.9
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	10	28.9
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	10	28.9
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	10	28.9
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	10	28.9
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	10	28.9
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	13	28.75
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	13	28.75
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	13	28.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	13	28.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	13	28.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	13	28.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	13	28.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	13	28.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	13	28.75
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	4	28.66
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	4	28.66
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	4	28.66
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	4	28.66
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	4	28.66
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	4	28.66
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	4	28.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	4	28.66
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	4	28.66
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	6	28.52
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	6	28.52
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	6	28.52
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	6	28.52
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	6	28.52
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	6	28.52
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	6	28.52
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	6	28.52
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	6	28.52
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	3	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	3	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	3	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	3	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	3	28.36
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	3	28.36
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	3	28.36
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	3	28.36
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	3	28.36
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	9	28.3
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	9	28.3
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	9	28.3
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	9	28.3
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	9	28.3
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	9	28.3
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	9	28.3
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	9	28.3
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	9	28.3
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	14	28.1
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	14	28.1
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	14	28.1
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	14	28.1
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	14	28.1
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	14	28.1
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	14	28.1
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	14	28.1
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	14	28.1
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.09
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.09
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.09
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.09
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.09
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	15	28.09
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	15	28.09
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	15	28.09
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	11	27.96
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	11	27.96
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	11	27.96
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	11	27.96
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	11	27.96
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	11	27.96
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	11	27.96
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	11	27.96
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	11	27.96
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	1	27.75
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	1	27.75
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	1	27.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	1	27.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	1	27.75
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	1	27.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	1	27.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	1	27.75
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	1	27.75
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	2	27.59
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	2	27.59
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	2	27.59
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	2	27.59
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	2	27.59
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	2	27.59
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	2	27.59
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	2	27.59
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	2	27.59
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	5	27.57
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	5	27.57
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	5	27.57
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	5	27.57
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	5	27.57
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	5	27.57
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	5	27.57
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	5	27.57
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	5	27.57
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG21	8	27.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG22	8	27.54
(2,114)	1:781:A:ILE:H	1:746:A:ILE:HG23	8	27.54
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG21	8	27.54
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG22	8	27.54
(2,113)	1:781:A:ILE:H	1:746:A:ILE:HG23	8	27.54
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG21	8	27.54
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG22	8	27.54
(2,112)	1:781:A:ILE:H	1:746:A:ILE:HG23	8	27.54
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	7	27.1
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	7	27.1
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	7	27.1
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	7	27.1
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	7	27.1
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	7	27.1
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	7	27.1
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	7	27.1
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	7	27.1
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	2	26.92
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	2	26.92
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	2	26.92
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	2	26.92
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	2	26.92
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	2	26.92
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	2	26.92
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	2	26.92
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	2	26.92
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	12	26.82
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	12	26.82
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	12	26.82
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	12	26.82
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	12	26.82
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	12	26.82
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	12	26.82
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	12	26.82
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	12	26.82
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	7	26.81
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	7	26.81
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	7	26.81
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	7	26.81
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	7	26.81
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	7	26.81
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	7	26.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	7	26.81
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	7	26.81
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	10	26.75
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	10	26.75
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	10	26.75
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	10	26.75
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	10	26.75
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	10	26.75
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	10	26.75
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	10	26.75
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	10	26.75
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	12	26.69
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	12	26.69
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	12	26.69
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	12	26.69
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	12	26.69
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	12	26.69
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	12	26.69
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	12	26.69
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	12	26.69
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	1	26.67
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	1	26.67
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	1	26.67
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	10	26.67
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	10	26.67
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	10	26.67
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	1	26.67
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	1	26.67
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	1	26.67
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	10	26.67
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	10	26.67
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	10	26.67
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	1	26.67
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	1	26.67
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	1	26.67
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	10	26.67
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	10	26.67
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	10	26.67
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	8	26.5
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	8	26.5
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	8	26.5
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	8	26.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	8	26.5
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	8	26.5
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	8	26.5
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	8	26.5
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	8	26.5
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	3	26.32
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	3	26.32
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	3	26.32
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	3	26.32
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	3	26.32
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	3	26.32
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	3	26.32
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	3	26.32
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	3	26.32
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	2	26.2
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	2	26.2
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	2	26.2
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	2	26.2
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	2	26.2
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	2	26.2
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	2	26.2
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	2	26.2
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	2	26.2
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	13	26.19
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	13	26.19
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	13	26.19
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	13	26.19
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	13	26.19
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	13	26.19
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	13	26.19
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	13	26.19
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	13	26.19
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	13	26.17
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	13	26.17
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	13	26.17
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	13	26.17
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	13	26.17
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	13	26.17
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	13	26.17
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	13	26.17
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	13	26.17
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	11	26.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	11	26.15
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	11	26.15
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	11	26.15
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	11	26.15
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	11	26.15
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	11	26.15
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	11	26.15
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	11	26.15
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	1	26.14
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	1	26.14
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	1	26.14
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	1	26.14
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	1	26.14
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	1	26.14
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	1	26.14
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	1	26.14
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	1	26.14
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	10	26.13
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	10	26.13
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	10	26.13
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	10	26.13
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	10	26.13
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	10	26.13
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	10	26.13
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	10	26.13
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	10	26.13
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	12	26.0
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	12	26.0
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	12	26.0
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	12	26.0
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	12	26.0
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	12	26.0
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	12	26.0
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	12	26.0
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	12	26.0
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	7	26.0
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	7	26.0
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	7	26.0
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	7	26.0
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	7	26.0
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	7	26.0
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	7	26.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	7	26.0
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	7	26.0
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	5	25.97
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	5	25.97
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	5	25.97
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	5	25.97
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	5	25.97
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	5	25.97
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	5	25.97
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	5	25.97
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	5	25.97
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	14	25.96
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	14	25.96
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	14	25.96
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	14	25.96
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	14	25.96
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	14	25.96
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	14	25.96
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	14	25.96
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	14	25.96
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	8	25.81
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	8	25.81
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	8	25.81
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	8	25.81
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	8	25.81
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	8	25.81
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	8	25.81
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	8	25.81
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	8	25.81
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	3	25.79
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	3	25.79
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	3	25.79
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	3	25.79
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	3	25.79
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	3	25.79
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	3	25.79
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	3	25.79
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	3	25.79
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	4	25.75
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	4	25.75
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	4	25.75
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	4	25.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	4	25.75
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	4	25.75
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	4	25.75
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	4	25.75
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	4	25.75
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	11	25.7
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	11	25.7
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	11	25.7
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	11	25.7
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	11	25.7
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	11	25.7
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	11	25.7
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	11	25.7
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	11	25.7
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	9	25.68
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	9	25.68
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	9	25.68
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	9	25.68
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	9	25.68
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	9	25.68
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	9	25.68
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	9	25.68
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	9	25.68
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	4	25.61
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	4	25.61
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	4	25.61
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	4	25.61
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	4	25.61
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	4	25.61
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	4	25.61
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	4	25.61
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	4	25.61
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	13	25.6
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	13	25.6
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	13	25.6
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	13	25.6
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	13	25.6
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	13	25.6
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	13	25.6
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	13	25.6
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	13	25.6
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	14	25.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	14	25.57
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	14	25.57
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	14	25.57
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	14	25.57
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	14	25.57
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	14	25.57
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	14	25.57
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	14	25.57
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	11	25.47
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	11	25.47
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	11	25.47
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	11	25.47
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	11	25.47
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	11	25.47
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	11	25.47
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	11	25.47
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	11	25.47
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	1	25.44
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	1	25.44
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	1	25.44
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	1	25.44
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	1	25.44
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	1	25.44
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	1	25.44
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	1	25.44
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	1	25.44
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	6	25.44
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	6	25.44
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	6	25.44
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	6	25.44
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	6	25.44
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	6	25.44
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	6	25.44
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	6	25.44
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	6	25.44
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	9	25.43
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	9	25.43
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	9	25.43
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	9	25.43
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	9	25.43
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	9	25.43
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	9	25.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	9	25.43
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	9	25.43
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	6	25.36
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	6	25.36
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	6	25.36
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	6	25.36
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	6	25.36
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	6	25.36
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	6	25.36
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	6	25.36
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	6	25.36
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	5	25.32
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	5	25.32
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	5	25.32
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	5	25.32
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	5	25.32
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	5	25.32
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	5	25.32
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	5	25.32
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	5	25.32
(2,93)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	25.29
(2,93)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	25.29
(2,93)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	25.29
(2,92)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	25.29
(2,92)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	25.29
(2,92)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	25.29
(2,91)	1:749:A:VAL:HG11	1:782:A:VAL:H	15	25.29
(2,91)	1:749:A:VAL:HG12	1:782:A:VAL:H	15	25.29
(2,91)	1:749:A:VAL:HG13	1:782:A:VAL:H	15	25.29
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	3	25.19
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	3	25.19
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	3	25.19
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	3	25.19
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	3	25.19
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	3	25.19
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	3	25.19
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	3	25.19
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	3	25.19
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	14	25.14
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	14	25.14
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	14	25.14
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	14	25.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	14	25.14
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	14	25.14
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	14	25.14
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	14	25.14
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	14	25.14
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.13
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.13
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.13
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.13
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.13
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.13
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	15	25.13
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	15	25.13
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	15	25.13
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	8	25.12
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	8	25.12
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	8	25.12
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	8	25.12
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	8	25.12
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	8	25.12
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	8	25.12
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	8	25.12
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	8	25.12
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.08
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.08
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.08
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.08
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.08
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.08
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	15	25.08
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	15	25.08
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	15	25.08
(2,117)	1:781:A:ILE:HD11	1:743:A:ASP:HA	5	25.05
(2,117)	1:781:A:ILE:HD12	1:743:A:ASP:HA	5	25.05
(2,117)	1:781:A:ILE:HD13	1:743:A:ASP:HA	5	25.05
(2,116)	1:781:A:ILE:HD11	1:743:A:ASP:HA	5	25.05
(2,116)	1:781:A:ILE:HD12	1:743:A:ASP:HA	5	25.05
(2,116)	1:781:A:ILE:HD13	1:743:A:ASP:HA	5	25.05
(2,115)	1:781:A:ILE:HD11	1:743:A:ASP:HA	5	25.05
(2,115)	1:781:A:ILE:HD12	1:743:A:ASP:HA	5	25.05
(2,115)	1:781:A:ILE:HD13	1:743:A:ASP:HA	5	25.05
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	4	24.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	4	24.96
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	4	24.96
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	4	24.96
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	4	24.96
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	4	24.96
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	4	24.93
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	4	24.93
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	4	24.93
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	4	24.93
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	4	24.93
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	4	24.93
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	4	24.93
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	4	24.93
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	4	24.93
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	7	24.91
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	7	24.91
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	7	24.91
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	7	24.91
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	7	24.91
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	7	24.91
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	7	24.91
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	7	24.91
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	7	24.91
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	7	24.91
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	7	24.91
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	7	24.91
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	7	24.91
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	7	24.91
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	7	24.91
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	7	24.91
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	7	24.91
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	7	24.91
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	6	24.84
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	6	24.84
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	6	24.84
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	6	24.84
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	6	24.84
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	6	24.84
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	6	24.84
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	6	24.84
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	6	24.84
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	13	24.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	13	24.77
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	13	24.77
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	13	24.77
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	13	24.77
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	13	24.77
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	13	24.77
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	13	24.77
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	13	24.77
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	13	24.77
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	13	24.77
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	13	24.77
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	13	24.77
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	13	24.77
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	13	24.77
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	13	24.77
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	13	24.77
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	13	24.77
(2,129)	1:785:A:LEU:HD21	1:749:A:VAL:HB	9	24.74
(2,129)	1:785:A:LEU:HD22	1:749:A:VAL:HB	9	24.74
(2,129)	1:785:A:LEU:HD23	1:749:A:VAL:HB	9	24.74
(2,128)	1:785:A:LEU:HD21	1:749:A:VAL:HB	9	24.74
(2,128)	1:785:A:LEU:HD22	1:749:A:VAL:HB	9	24.74
(2,128)	1:785:A:LEU:HD23	1:749:A:VAL:HB	9	24.74
(2,127)	1:785:A:LEU:HD21	1:749:A:VAL:HB	9	24.74
(2,127)	1:785:A:LEU:HD22	1:749:A:VAL:HB	9	24.74
(2,127)	1:785:A:LEU:HD23	1:749:A:VAL:HB	9	24.74
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	11	24.7
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	11	24.7
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	11	24.7
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	11	24.7
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	11	24.7
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	11	24.7
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	11	24.7
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	11	24.7
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	11	24.7
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	11	24.7
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	11	24.7
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	11	24.7
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	11	24.7
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	11	24.7
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	11	24.7
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	11	24.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	11	24.7
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	11	24.7
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	11	24.59
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	11	24.59
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	11	24.59
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	11	24.59
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	11	24.59
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	11	24.59
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	8	24.49
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	8	24.49
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	8	24.49
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	8	24.49
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	8	24.49
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	8	24.49
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	8	24.49
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	8	24.49
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	8	24.49
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	8	24.49
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	8	24.49
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	8	24.49
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	8	24.49
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	8	24.49
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	8	24.49
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	8	24.49
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	8	24.49
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	8	24.49
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	12	24.47
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	12	24.47
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	12	24.47
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	12	24.47
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	12	24.47
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	12	24.47
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	9	24.45
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	9	24.45
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	9	24.45
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	9	24.45
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	9	24.45
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	9	24.45
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	9	24.45
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	9	24.45
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	9	24.45
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	9	24.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	9	24.45
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	9	24.45
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	9	24.45
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	9	24.45
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	9	24.45
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	9	24.45
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	9	24.45
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	9	24.45
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	4	24.42
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	4	24.42
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	4	24.42
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	4	24.42
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	4	24.42
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	4	24.42
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.42
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.42
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.42
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.42
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.42
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.42
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	4	24.42
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	4	24.42
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	4	24.42
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	4	24.42
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	4	24.42
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	4	24.42
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.42
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.42
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.42
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.42
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.42
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.42
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	4	24.42
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	4	24.42
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	4	24.42
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	4	24.42
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	4	24.42
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	4	24.42
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	15	24.42
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	15	24.42
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	15	24.42
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	15	24.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	15	24.42
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	15	24.42
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	5	24.38
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	5	24.38
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	5	24.38
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	5	24.38
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	5	24.38
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	5	24.38
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	5	24.38
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	5	24.38
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	5	24.38
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	5	24.38
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	5	24.38
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	5	24.38
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	5	24.38
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	5	24.38
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	5	24.38
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	5	24.38
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	5	24.38
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	5	24.38
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	10	24.32
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	10	24.32
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	10	24.32
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	10	24.32
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	10	24.32
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	10	24.32
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	10	24.32
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	10	24.32
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	10	24.32
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	10	24.32
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	10	24.32
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	10	24.32
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	10	24.32
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	10	24.32
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	10	24.32
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	10	24.32
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	10	24.32
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	10	24.32
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	3	24.31
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	3	24.31
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	3	24.31
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	3	24.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	3	24.31
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	3	24.31
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	3	24.31
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	3	24.31
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	3	24.31
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	3	24.31
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	3	24.31
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	3	24.31
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	3	24.31
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	3	24.31
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	3	24.31
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	3	24.31
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	3	24.31
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	3	24.31
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	8	24.31
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	8	24.31
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	8	24.31
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	8	24.31
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	8	24.31
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	8	24.31
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	2	24.29
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	2	24.29
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	2	24.29
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	2	24.29
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	2	24.29
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	2	24.29
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	2	24.29
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	2	24.29
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	2	24.29
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	2	24.29
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	2	24.29
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	2	24.29
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	2	24.29
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	2	24.29
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	2	24.29
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	2	24.29
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	2	24.29
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	2	24.29
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	12	24.26
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	12	24.26
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	12	24.26
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	12	24.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	12	24.26
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	12	24.26
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	12	24.26
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	12	24.26
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	12	24.26
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	12	24.26
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	12	24.26
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	12	24.26
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	12	24.26
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	12	24.26
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	12	24.26
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	12	24.26
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	12	24.26
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	12	24.26
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	7	24.26
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	7	24.26
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	7	24.26
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	7	24.26
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	7	24.26
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	7	24.26
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	3	24.13
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	3	24.13
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	3	24.13
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	3	24.13
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	3	24.13
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	3	24.13
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	2	24.06
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	2	24.06
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	2	24.06
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	2	24.06
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	2	24.06
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	2	24.06
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	2	24.06
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	2	24.06
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	2	24.06
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	2	24.06
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	2	24.06
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	2	24.06
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	2	24.06
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	2	24.06
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	2	24.06
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	2	24.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	2	24.06
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	2	24.06
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	9	24.01
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	9	24.01
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	9	24.01
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	9	24.01
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	9	24.01
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	9	24.01
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	5	23.91
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	5	23.91
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	5	23.91
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	5	23.91
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	5	23.91
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	5	23.91
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	13	23.89
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	13	23.89
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	13	23.89
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	13	23.89
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	13	23.89
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	13	23.89
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	1	23.85
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	1	23.85
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	1	23.85
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	1	23.85
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	1	23.85
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	1	23.85
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	1	23.85
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	1	23.85
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	1	23.85
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	1	23.85
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	1	23.85
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	1	23.85
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	1	23.85
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	1	23.85
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	1	23.85
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	1	23.85
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	1	23.85
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	1	23.85
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.79
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.79
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.79
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	15	23.79
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	15	23.79
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	6	23.76
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	6	23.76
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	6	23.76
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	6	23.76
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	6	23.76
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	6	23.76
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	6	23.76
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	6	23.76
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	6	23.76
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	6	23.76
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	6	23.76
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	6	23.76
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	6	23.76
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	6	23.76
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	6	23.76
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	6	23.76
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	6	23.76
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	6	23.76
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	6	23.74
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	6	23.74
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	6	23.74
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	6	23.74
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	6	23.74
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	6	23.74
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	10	23.72
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	10	23.72
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	10	23.72
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	10	23.72
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	10	23.72
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	10	23.72
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	10	23.72
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	10	23.72
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	10	23.72
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	10	23.72
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	10	23.72
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	10	23.72
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	10	23.72
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	10	23.72
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	10	23.72
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	10	23.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	10	23.72
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	10	23.72
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	10	23.64
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	10	23.64
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	10	23.64
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	10	23.64
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	10	23.64
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	10	23.64
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	2	23.37
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	2	23.37
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	2	23.37
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	2	23.37
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	2	23.37
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	2	23.37
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	7	23.24
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	7	23.24
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	7	23.24
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	7	23.24
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	7	23.24
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	7	23.24
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	7	23.24
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	7	23.24
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	7	23.24
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	7	23.24
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	7	23.24
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	7	23.24
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	7	23.24
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	7	23.24
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	7	23.24
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	7	23.24
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	7	23.24
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	7	23.24
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	1	23.24
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	1	23.24
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	1	23.24
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	1	23.24
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	1	23.24
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	1	23.24
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	10	23.22
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	10	23.22
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	10	23.22
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	10	23.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	10	23.22
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	10	23.22
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	10	23.22
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	10	23.22
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	10	23.22
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	10	23.22
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	10	23.22
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	10	23.22
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	10	23.22
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	10	23.22
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	10	23.22
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	10	23.22
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	10	23.22
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	10	23.22
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	8	23.06
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	8	23.06
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	8	23.06
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	8	23.06
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	8	23.06
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	8	23.06
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	7	23.05
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	7	23.05
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	7	23.05
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	7	23.05
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	7	23.05
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	7	23.05
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	7	23.05
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	7	23.05
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	7	23.05
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	7	23.05
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	7	23.05
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	7	23.05
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	7	23.05
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	7	23.05
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	7	23.05
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	7	23.05
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	7	23.05
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	7	23.05
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	1	23.04
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	1	23.04
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	1	23.04
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	1	23.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	1	23.04
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	1	23.04
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	1	23.04
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	1	23.04
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	1	23.04
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	1	23.04
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	1	23.04
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	1	23.04
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	1	23.04
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	1	23.04
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	1	23.04
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	1	23.04
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	1	23.04
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	1	23.04
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	12	22.96
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	12	22.96
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	12	22.96
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	12	22.96
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	12	22.96
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	12	22.96
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	12	22.96
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	12	22.96
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	12	22.96
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	12	22.96
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	12	22.96
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	12	22.96
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	12	22.96
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	12	22.96
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	12	22.96
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	12	22.96
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	12	22.96
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	12	22.96
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.92
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.92
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.92
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.92
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	15	22.92
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	15	22.92
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	14	22.9
(2,111)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	14	22.9
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	14	22.9
(2,111)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	14	22.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	14	22.9
(2,111)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	14	22.9
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	14	22.9
(2,110)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	14	22.9
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	14	22.9
(2,110)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	14	22.9
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	14	22.9
(2,110)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	14	22.9
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD2	14	22.9
(2,109)	1:777:A:ILE:HD11	1:742:A:ARG:HD3	14	22.9
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD2	14	22.9
(2,109)	1:777:A:ILE:HD12	1:742:A:ARG:HD3	14	22.9
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD2	14	22.9
(2,109)	1:777:A:ILE:HD13	1:742:A:ARG:HD3	14	22.9
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD2	14	22.84
(2,108)	1:763:A:LEU:H	1:742:A:ARG:HD3	14	22.84
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD2	14	22.84
(2,107)	1:763:A:LEU:H	1:742:A:ARG:HD3	14	22.84
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD2	14	22.84
(2,106)	1:763:A:LEU:H	1:742:A:ARG:HD3	14	22.84
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	5	22.83
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	5	22.83
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	5	22.83
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	5	22.83
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	5	22.83
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	5	22.83
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	6	22.82
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	6	22.82
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	6	22.82
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	6	22.82
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	6	22.82
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	6	22.82
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	6	22.82
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	6	22.82
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	6	22.82
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	6	22.82
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	6	22.82
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	6	22.82
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	6	22.82
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	6	22.82
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	6	22.82
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	6	22.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	6	22.82
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	6	22.82
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	11	22.79
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	11	22.79
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	11	22.79
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	11	22.79
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	11	22.79
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	11	22.79
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	4	22.78
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	4	22.78
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	4	22.78
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	4	22.78
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	4	22.78
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	4	22.78
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	4	22.78
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	4	22.78
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	4	22.78
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	4	22.78
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	4	22.78
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	4	22.78
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	4	22.78
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	4	22.78
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	4	22.78
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	4	22.78
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	4	22.78
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	4	22.78
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	13	22.77
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	13	22.77
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	13	22.77
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	13	22.77
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	13	22.77
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	13	22.77
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	13	22.77
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	13	22.77
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	13	22.77
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	13	22.77
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	13	22.77
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	13	22.77
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	13	22.77
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	13	22.77
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	13	22.77
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	13	22.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	13	22.77
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	13	22.77
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	6	22.63
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	6	22.63
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	6	22.63
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	6	22.63
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	6	22.63
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	6	22.63
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	6	22.63
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	6	22.63
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	6	22.63
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	6	22.63
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	6	22.63
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	6	22.63
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	6	22.63
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	6	22.63
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	6	22.63
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	6	22.63
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	6	22.63
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	6	22.63
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	12	22.58
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	12	22.58
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	12	22.58
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	12	22.58
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	12	22.58
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	12	22.58
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	8	22.55
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	8	22.55
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	8	22.55
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	8	22.55
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	8	22.55
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	8	22.55
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	8	22.55
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	8	22.55
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	8	22.55
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	8	22.55
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	8	22.55
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	8	22.55
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	8	22.55
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	8	22.55
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	8	22.55
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	8	22.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	8	22.55
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	8	22.55
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	10	22.5
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	10	22.5
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	10	22.5
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	10	22.5
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	10	22.5
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	10	22.5
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	14	22.48
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	14	22.48
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	14	22.48
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	14	22.48
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	14	22.48
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	14	22.48
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	14	22.48
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	14	22.48
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	14	22.48
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	14	22.48
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	14	22.48
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	14	22.48
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	14	22.48
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	14	22.48
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	14	22.48
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	14	22.48
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	14	22.48
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	14	22.48
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	3	22.43
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	3	22.43
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	3	22.43
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	3	22.43
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	3	22.43
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	3	22.43
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	3	22.43
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	3	22.43
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	3	22.43
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	3	22.43
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	3	22.43
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	3	22.43
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	3	22.43
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	3	22.43
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	3	22.43
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	3	22.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	3	22.43
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	3	22.43
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	14	22.36
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	14	22.36
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	14	22.36
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	14	22.36
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	14	22.36
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	14	22.36
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	11	22.35
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	11	22.35
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	11	22.35
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	11	22.35
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	11	22.35
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	11	22.35
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	11	22.35
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	11	22.35
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	11	22.35
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	11	22.35
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	11	22.35
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	11	22.35
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	11	22.35
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	11	22.35
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	11	22.35
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	11	22.35
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	11	22.35
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	11	22.35
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	9	22.29
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	9	22.29
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	9	22.29
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	9	22.29
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	9	22.29
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	9	22.29
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	9	22.29
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	9	22.29
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	9	22.29
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	9	22.29
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	9	22.29
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	9	22.29
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	9	22.29
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	9	22.29
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	9	22.29
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	9	22.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	9	22.29
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	9	22.29
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	3	22.28
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	3	22.28
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	3	22.28
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	3	22.28
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	3	22.28
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	3	22.28
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	6	22.24
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	6	22.24
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	6	22.24
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	6	22.24
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	6	22.24
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	6	22.24
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	1	22.14
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	1	22.14
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	1	22.14
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	1	22.14
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	1	22.14
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	1	22.14
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	1	22.14
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	1	22.14
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	1	22.14
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	1	22.14
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	1	22.14
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	1	22.14
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	1	22.14
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	1	22.14
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	1	22.14
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	1	22.14
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	1	22.14
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	1	22.14
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	13	22.1
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	13	22.1
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	13	22.1
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	13	22.1
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	13	22.1
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	13	22.1
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	13	22.1
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	13	22.1
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	13	22.1
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	13	22.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	13	22.1
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	13	22.1
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	13	22.1
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	13	22.1
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	13	22.1
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	13	22.1
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	13	22.1
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	13	22.1
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	12	22.08
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	12	22.08
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	12	22.08
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	12	22.08
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	12	22.08
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	12	22.08
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	12	22.08
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	12	22.08
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	12	22.08
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	12	22.08
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	12	22.08
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	12	22.08
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	12	22.08
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	12	22.08
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	12	22.08
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	12	22.08
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	12	22.08
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	12	22.08
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	9	22.04
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	9	22.04
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	9	22.04
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	9	22.04
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	9	22.04
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	9	22.04
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	2	22.0
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	2	22.0
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	2	22.0
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	2	22.0
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	2	22.0
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	2	22.0
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	2	22.0
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	2	22.0
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	2	22.0
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	2	22.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	2	22.0
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	2	22.0
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	2	22.0
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	2	22.0
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	2	22.0
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	2	22.0
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	2	22.0
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	2	22.0
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	13	21.97
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	13	21.97
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	13	21.97
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	13	21.97
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	13	21.97
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	13	21.97
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	13	21.84
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	13	21.84
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	13	21.84
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	13	21.84
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	13	21.84
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	13	21.84
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	13	21.84
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	13	21.84
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	13	21.84
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	13	21.84
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	13	21.84
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	13	21.84
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	13	21.84
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	13	21.84
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	13	21.84
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	13	21.84
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	13	21.84
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	13	21.84
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.83
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.83
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.83
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.83
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.83
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.83
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.83
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.83
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.83
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.83
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.83
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	15	21.83
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	15	21.83
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	15	21.83
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	15	21.83
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	15	21.83
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	15	21.83
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	2	21.8
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	2	21.8
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	2	21.8
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	2	21.8
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	2	21.8
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	2	21.8
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	1	21.79
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	1	21.79
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	1	21.79
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	1	21.79
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	1	21.79
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	1	21.79
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	10	21.75
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	10	21.75
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	10	21.75
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	10	21.75
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	10	21.75
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	10	21.75
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	10	21.75
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	10	21.75
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	10	21.75
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	10	21.75
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	10	21.75
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	10	21.75
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	10	21.75
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	10	21.75
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	10	21.75
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	10	21.75
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	10	21.75
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	10	21.75
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	12	21.73
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	12	21.73
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	12	21.73
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	12	21.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	12	21.73
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	12	21.73
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	12	21.73
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	12	21.73
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	12	21.73
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	12	21.73
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	12	21.73
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	12	21.73
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	12	21.73
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	12	21.73
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	12	21.73
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	12	21.73
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	12	21.73
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	12	21.73
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	21.73
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	21.73
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	21.73
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	21.73
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	21.73
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	21.73
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	21.73
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	21.73
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	21.73
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	21.73
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	21.73
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	21.73
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	15	21.73
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	15	21.73
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	15	21.73
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	15	21.73
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	15	21.73
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	15	21.73
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	7	21.59
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	7	21.59
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	7	21.59
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	7	21.59
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	7	21.59
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	7	21.59
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	7	21.59
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	7	21.59
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	7	21.59
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	7	21.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	7	21.59
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	7	21.59
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	7	21.59
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	7	21.59
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	7	21.59
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	7	21.59
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	7	21.59
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	7	21.59
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	4	21.59
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	4	21.59
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	4	21.59
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	4	21.59
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	4	21.59
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	4	21.59
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	5	21.58
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	5	21.58
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	5	21.58
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	5	21.58
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	5	21.58
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	5	21.58
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	5	21.58
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	5	21.58
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	5	21.58
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	5	21.58
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	5	21.58
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	5	21.58
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	5	21.58
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	5	21.58
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	5	21.58
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	5	21.58
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	5	21.58
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	5	21.58
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB2	7	21.56
(2,96)	1:754:A:ALA:H	1:716:A:SER:HB3	7	21.56
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB2	7	21.56
(2,95)	1:754:A:ALA:H	1:716:A:SER:HB3	7	21.56
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB2	7	21.56
(2,94)	1:754:A:ALA:H	1:716:A:SER:HB3	7	21.56
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	3	21.52
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	3	21.52
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	3	21.52
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	3	21.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	3	21.52
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	3	21.52
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	3	21.52
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	3	21.52
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	3	21.52
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	3	21.52
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	3	21.52
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	3	21.52
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	3	21.52
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	3	21.52
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	3	21.52
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	3	21.52
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	3	21.52
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	3	21.52
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	14	21.48
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	14	21.48
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	14	21.48
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	14	21.48
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	14	21.48
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	14	21.48
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	14	21.48
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	14	21.48
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	14	21.48
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	14	21.48
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	14	21.48
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	14	21.48
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	14	21.48
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	14	21.48
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	14	21.48
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	14	21.48
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	14	21.48
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	14	21.48
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	11	21.34
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	11	21.34
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	11	21.34
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	11	21.34
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	11	21.34
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	11	21.34
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	11	21.34
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	11	21.34
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	11	21.34
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	11	21.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	11	21.34
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	11	21.34
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	11	21.34
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	11	21.34
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	11	21.34
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	11	21.34
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	11	21.34
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	11	21.34
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	5	21.31
(2,120)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	5	21.31
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	5	21.31
(2,120)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	5	21.31
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	5	21.31
(2,120)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	5	21.31
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	5	21.31
(2,119)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	5	21.31
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	5	21.31
(2,119)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	5	21.31
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	5	21.31
(2,119)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	5	21.31
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG12	5	21.31
(2,118)	1:781:A:ILE:HD11	1:746:A:ILE:HG13	5	21.31
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG12	5	21.31
(2,118)	1:781:A:ILE:HD12	1:746:A:ILE:HG13	5	21.31
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG12	5	21.31
(2,118)	1:781:A:ILE:HD13	1:746:A:ILE:HG13	5	21.31
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	9	21.19
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	9	21.19
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	9	21.19
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	9	21.19
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	9	21.19
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	9	21.19
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	9	21.19
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	9	21.19
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	9	21.19
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	9	21.19
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	9	21.19
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	9	21.19
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	9	21.19
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	9	21.19
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	9	21.19
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	9	21.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	9	21.19
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	9	21.19
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	5	21.18
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	5	21.18
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	5	21.18
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	5	21.18
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	5	21.18
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	5	21.18
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	5	21.18
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	5	21.18
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	5	21.18
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	5	21.18
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	5	21.18
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	5	21.18
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	5	21.18
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	5	21.18
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	5	21.18
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	5	21.18
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	5	21.18
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	5	21.18
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	6	21.13
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	6	21.13
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	6	21.13
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	6	21.13
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	6	21.13
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	6	21.13
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	6	21.13
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	6	21.13
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	6	21.13
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	6	21.13
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	6	21.13
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	6	21.13
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	6	21.13
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	6	21.13
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	6	21.13
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	6	21.13
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	6	21.13
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	6	21.13
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	4	21.07
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	4	21.07
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	4	21.07
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	4	21.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	4	21.07
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	4	21.07
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	4	21.07
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	4	21.07
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	4	21.07
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	4	21.07
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	4	21.07
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	4	21.07
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	4	21.07
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	4	21.07
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	4	21.07
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	4	21.07
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	4	21.07
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	4	21.07
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.02
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.02
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.02
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.02
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.02
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.02
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.02
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.02
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.02
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.02
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.02
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.02
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	15	21.02
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	15	21.02
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	15	21.02
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	15	21.02
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	15	21.02
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	15	21.02
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	8	21.01
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	8	21.01
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	8	21.01
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	8	21.01
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	8	21.01
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	8	21.01
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	8	21.01
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	8	21.01
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	8	21.01
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	8	21.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	8	21.01
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	8	21.01
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	8	21.01
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	8	21.01
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	8	21.01
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	8	21.01
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	8	21.01
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	8	21.01
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	1	20.99
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	1	20.99
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	1	20.99
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	1	20.99
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	1	20.99
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	1	20.99
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	1	20.99
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	1	20.99
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	1	20.99
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	1	20.99
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	1	20.99
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	1	20.99
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	1	20.99
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	1	20.99
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	1	20.99
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	1	20.99
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	1	20.99
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	1	20.99
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	14	20.98
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	14	20.98
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	14	20.98
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	14	20.98
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	14	20.98
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	14	20.98
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	14	20.98
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	14	20.98
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	14	20.98
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	14	20.98
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	14	20.98
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	14	20.98
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	14	20.98
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	14	20.98
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	14	20.98
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	14	20.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	14	20.98
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	14	20.98
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	2	20.87
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	2	20.87
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	2	20.87
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	2	20.87
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	2	20.87
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	2	20.87
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	2	20.87
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	2	20.87
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	2	20.87
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	2	20.87
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	2	20.87
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	2	20.87
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	2	20.87
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	2	20.87
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	2	20.87
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	2	20.87
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	2	20.87
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	2	20.87
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB2	4	20.81
(2,123)	1:785:A:LEU:HD21	1:716:A:SER:HB3	4	20.81
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB2	4	20.81
(2,123)	1:785:A:LEU:HD22	1:716:A:SER:HB3	4	20.81
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB2	4	20.81
(2,123)	1:785:A:LEU:HD23	1:716:A:SER:HB3	4	20.81
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB2	4	20.81
(2,122)	1:785:A:LEU:HD21	1:716:A:SER:HB3	4	20.81
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB2	4	20.81
(2,122)	1:785:A:LEU:HD22	1:716:A:SER:HB3	4	20.81
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB2	4	20.81
(2,122)	1:785:A:LEU:HD23	1:716:A:SER:HB3	4	20.81
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB2	4	20.81
(2,121)	1:785:A:LEU:HD21	1:716:A:SER:HB3	4	20.81
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB2	4	20.81
(2,121)	1:785:A:LEU:HD22	1:716:A:SER:HB3	4	20.81
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB2	4	20.81
(2,121)	1:785:A:LEU:HD23	1:716:A:SER:HB3	4	20.81
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	9	20.74
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	9	20.74
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	9	20.74
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	9	20.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	9	20.74
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	9	20.74
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	9	20.74
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	9	20.74
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	9	20.74
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	9	20.74
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	9	20.74
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	9	20.74
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	9	20.74
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	9	20.74
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	9	20.74
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	9	20.74
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	9	20.74
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	9	20.74
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	3	20.34
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	3	20.34
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	3	20.34
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	3	20.34
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	3	20.34
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	3	20.34
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	3	20.34
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	3	20.34
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	3	20.34
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	3	20.34
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	3	20.34
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	3	20.34
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	3	20.34
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	3	20.34
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	3	20.34
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	3	20.34
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	3	20.34
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	3	20.34
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	11	19.36
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	11	19.36
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	11	19.36
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	11	19.36
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	11	19.36
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	11	19.36
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	11	19.36
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	11	19.36
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	11	19.36
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	11	19.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	11	19.36
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	11	19.36
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	11	19.36
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	11	19.36
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	11	19.36
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	11	19.36
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	11	19.36
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	11	19.36
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	8	19.1
(2,126)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	8	19.1
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	8	19.1
(2,126)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	8	19.1
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	8	19.1
(2,126)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	8	19.1
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	8	19.1
(2,125)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	8	19.1
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	8	19.1
(2,125)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	8	19.1
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	8	19.1
(2,125)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	8	19.1
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD2	8	19.1
(2,124)	1:785:A:LEU:HD21	1:747:A:ARG:HD3	8	19.1
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD2	8	19.1
(2,124)	1:785:A:LEU:HD22	1:747:A:ARG:HD3	8	19.1
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD2	8	19.1
(2,124)	1:785:A:LEU:HD23	1:747:A:ARG:HD3	8	19.1
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	11	17.93
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	11	17.93
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	11	17.93
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	11	17.93
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	11	17.93
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	11	17.93
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	11	17.93
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	11	17.93
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	11	17.93
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	17.92
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	17.92
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	17.92
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	17.92
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	17.92
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	17.92
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	15	17.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	15	17.92
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	15	17.92
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	8	17.44
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	8	17.44
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	8	17.44
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	8	17.44
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	8	17.44
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	8	17.44
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	8	17.44
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	8	17.44
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	8	17.44
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	14	17.41
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	14	17.41
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	14	17.41
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	14	17.41
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	14	17.41
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	14	17.41
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	14	17.41
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	14	17.41
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	14	17.41
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	5	17.34
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	5	17.34
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	5	17.34
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	5	17.34
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	5	17.34
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	5	17.34
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	5	17.34
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	5	17.34
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	5	17.34
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	4	17.08
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	4	17.08
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	4	17.08
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	4	17.08
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	4	17.08
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	4	17.08
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	4	17.08
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	4	17.08
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	4	17.08
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	12	16.99
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	12	16.99
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	12	16.99
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	12	16.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	12	16.99
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	12	16.99
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	12	16.99
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	12	16.99
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	12	16.99
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	9	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	9	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	9	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	9	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	9	16.8
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	9	16.8
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	9	16.8
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	9	16.8
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	9	16.8
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	3	16.78
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	3	16.78
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	3	16.78
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	3	16.78
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	3	16.78
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	3	16.78
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	3	16.78
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	3	16.78
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	3	16.78
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	6	16.75
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	6	16.75
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	6	16.75
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	6	16.75
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	6	16.75
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	6	16.75
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	6	16.75
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	6	16.75
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	6	16.75
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	2	16.71
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	2	16.71
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	2	16.71
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	2	16.71
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	2	16.71
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	2	16.71
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	2	16.71
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	2	16.71
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	2	16.71
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	10	16.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	10	16.7
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	10	16.7
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	10	16.7
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	10	16.7
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	10	16.7
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	10	16.7
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	10	16.7
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	10	16.7
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	1	16.67
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	1	16.67
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	1	16.67
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	1	16.67
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	1	16.67
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	1	16.67
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	1	16.67
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	1	16.67
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	1	16.67
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	13	16.48
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	13	16.48
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	13	16.48
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	13	16.48
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	13	16.48
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	13	16.48
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	13	16.48
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	13	16.48
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	13	16.48
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD21	7	15.83
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD22	7	15.83
(2,102)	1:758:A:ASP:H	1:715:A:LEU:HD23	7	15.83
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD21	7	15.83
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD22	7	15.83
(2,101)	1:758:A:ASP:H	1:715:A:LEU:HD23	7	15.83
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD21	7	15.83
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD22	7	15.83
(2,100)	1:758:A:ASP:H	1:715:A:LEU:HD23	7	15.83
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	8	14.28
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	8	14.28
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	8	14.28
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	8	14.28
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	8	14.28
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	8	14.28
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	14.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	14.11
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	14.11
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	14.11
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	15	14.11
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	15	14.11
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	6	14.08
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	6	14.08
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	6	14.08
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	6	14.08
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	6	14.08
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	6	14.08
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	8	14.05
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	8	14.05
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	8	14.05
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	8	14.05
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	8	14.05
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	8	14.05
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	10	14.04
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	10	14.04
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	10	14.04
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	10	14.04
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	10	14.04
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	10	14.04
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	11	13.99
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	11	13.99
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	11	13.99
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	11	13.99
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	11	13.99
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	11	13.99
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	5	13.89
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	5	13.89
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	5	13.89
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	5	13.89
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	5	13.89
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	5	13.89
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	3	13.72
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	3	13.72
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	3	13.72
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	3	13.72
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	3	13.72
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	3	13.72
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	4	13.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	4	13.7
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	4	13.7
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	4	13.7
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	4	13.7
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	4	13.7
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	14	13.67
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	14	13.67
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	14	13.67
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	14	13.67
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	14	13.67
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	14	13.67
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	9	13.66
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	9	13.66
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	9	13.66
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	9	13.66
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	9	13.66
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	9	13.66
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	2	13.58
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	2	13.58
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	2	13.58
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	2	13.58
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	2	13.58
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	2	13.58
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	13	13.57
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	13	13.57
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	13	13.57
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	13	13.57
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	13	13.57
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	13	13.57
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	1	13.49
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	1	13.49
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	1	13.49
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	1	13.49
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	1	13.49
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	1	13.49
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	12	13.23
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	12	13.23
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	12	13.23
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	12	13.23
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	12	13.23
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	12	13.23
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD2	7	13.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:759:A:ASP:H	1:709:A:ARG:HD3	7	13.13
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD2	7	13.13
(2,104)	1:759:A:ASP:H	1:709:A:ARG:HD3	7	13.13
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD2	7	13.13
(2,103)	1:759:A:ASP:H	1:709:A:ARG:HD3	7	13.13
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.88
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.88
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.88
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.88
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	15	12.88
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	15	12.88
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	5	12.77
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	5	12.77
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	5	12.77
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	5	12.77
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	5	12.77
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	5	12.77
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	12	12.73
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	12	12.73
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	12	12.73
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	12	12.73
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	12	12.73
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	12	12.73
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	10	12.68
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	10	12.68
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	10	12.68
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	10	12.68
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	10	12.68
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	10	12.68
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	3	12.67
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	3	12.67
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	3	12.67
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	3	12.67
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	3	12.67
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	3	12.67
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	6	12.63
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	6	12.63
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	6	12.63
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	6	12.63
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	6	12.63
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	6	12.63
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	11	12.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	11	12.54
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	11	12.54
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	11	12.54
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	11	12.54
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	11	12.54
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	14	12.4
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	14	12.4
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	14	12.4
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	14	12.4
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	14	12.4
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	14	12.4
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	4	12.32
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	4	12.32
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	4	12.32
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	4	12.32
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	4	12.32
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	4	12.32
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	13	12.21
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	13	12.21
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	13	12.21
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	13	12.21
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	13	12.21
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	13	12.21
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	7	12.14
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	7	12.14
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	7	12.14
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	7	12.14
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	7	12.14
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	7	12.14
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	9	12.04
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	9	12.04
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	9	12.04
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	9	12.04
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	9	12.04
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	9	12.04
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	2	12.02
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	2	12.02
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	2	12.02
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	2	12.02
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	2	12.02
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	2	12.02
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB2	1	11.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:711:A:GLY:H	1:758:A:ASP:HB3	1	11.94
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB2	1	11.94
(2,86)	1:711:A:GLY:H	1:758:A:ASP:HB3	1	11.94
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB2	1	11.94
(2,85)	1:711:A:GLY:H	1:758:A:ASP:HB3	1	11.94
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	10.06
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	10.06
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	10.06
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	10.06
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	10.06
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	10.06
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	10.06
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	10.06
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	10.06
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	9.9
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	9.9
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	9.9
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	9.9
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	9.9
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	9.9
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	9.9
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	9.9
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	9.9
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	9.9
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	9.9
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	9.9
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	15	9.9
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	15	9.9
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	15	9.9
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	15	9.9
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	15	9.9
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	15	9.9
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.54
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.54
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.5
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.5
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.5
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.5
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.5
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.5
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.5
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.5
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.5
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.34
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.34
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.34
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.34
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.34
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.34
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.34
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.34
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.34
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.31
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.31
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.31
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.31
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.31
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.31
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.31
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.31
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.31
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	9.24
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	9.24
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	9.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	9.2
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	9.2
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	9.2
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	9.2
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	9.2
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	9.2
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	9.2
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	9.2
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	9.2
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.13
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.13
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.13
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.09
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.09
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.09
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.07
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.07
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.07
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.07
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.07
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.07
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.05
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.05
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.05
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.05
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.05
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.05
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.05
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.05
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.05
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.04
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.04
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.03
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.03
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.03
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	9.03
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	9.03
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	9.03
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	9.03
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	9.03
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.01
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.01
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.01
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.99
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.99
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.99
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	8.98
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	8.98
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	8.98
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	8.98
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	8.98
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	8.98
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	8.98
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	8.98
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	8.98
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	8.98
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	8.98
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	8.98
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.94
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.94
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.94
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	8.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	8.9
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	8.9
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	8.9
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	8.9
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	8.9
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	8.9
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	8.9
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	8.9
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	8.85
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	8.85
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	8.85
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	8.82
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	8.82
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	8.82
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	8.78
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	8.78
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	8.78
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.77
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.77
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.77
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.74
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.74
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.74
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	8.72
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	8.72
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	8.72
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	8.72
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	8.72
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	8.72
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	8.72
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	8.72
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	8.72
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	8.65
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	8.65
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	8.65
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.64
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.64
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.64
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.64
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.64
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.64
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.63
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.63
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.49
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.49
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.49
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.49
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.49
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.49
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.4
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.4
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.4
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.4
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.4
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.4
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.24
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.24
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.24
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.24
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.24
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.24
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.07
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.07
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.07
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.07
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.07
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.07
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	7.93
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	7.93
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	7.93
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	7.93
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	7.93
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	7.93
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	7.82
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	7.82
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	7.82
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	7.82
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	7.82
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	7.82
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.72
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.72
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.72
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	7.72
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	7.72
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	7.68
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	7.68
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	7.68
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	7.68
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	7.68
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	7.68
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.67
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.67
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.67
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.67
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.67
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.67
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	7.66
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	7.66
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	7.66
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	7.66
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	7.66
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	7.66
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	7.65
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	7.65
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	7.65
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	7.49
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	7.49
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	7.49
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	7.49
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	15	7.49
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	15	7.49
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.45
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.45
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.45
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.45
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.45
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.45
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	3	7.4
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	3	7.4
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	3	7.4
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	3	7.4
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	3	7.4
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	3	7.4
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	3	7.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	3	7.4
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	3	7.4
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	3	7.4
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	3	7.4
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	3	7.4
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	3	7.4
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	3	7.4
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	3	7.4
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	3	7.4
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	3	7.4
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	3	7.4
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	7.37
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	7.37
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	7.37
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	7.37
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	7.37
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	7.37
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.31
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.31
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.31
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.31
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.31
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.31
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	11	7.26
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	11	7.26
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	11	7.26
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	11	7.26
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	11	7.26
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	11	7.26
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	11	7.26
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	11	7.26
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	11	7.26
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	12	7.22
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	12	7.22
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	12	7.22
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	12	7.22
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	12	7.22
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	12	7.22
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	12	7.22
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	12	7.22
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	12	7.22
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	12	7.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	12	7.22
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	12	7.22
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	12	7.22
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	12	7.22
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	12	7.22
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	12	7.22
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	12	7.22
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	12	7.22
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	7.04
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	7.04
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	7.04
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	7.04
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	7.04
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	7.04
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	15	7.04
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	15	7.04
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	15	7.04
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	5	6.97
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	5	6.97
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	5	6.97
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	5	6.97
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	5	6.97
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	5	6.97
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	5	6.97
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	5	6.97
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	5	6.97
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	5	6.97
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	5	6.97
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	5	6.97
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	5	6.97
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	5	6.97
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	5	6.97
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	5	6.97
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	5	6.97
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	5	6.97
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	12	6.94
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	12	6.94
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	12	6.94
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	12	6.94
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	12	6.94
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	12	6.94
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	12	6.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	12	6.94
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	12	6.94
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	10	6.84
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	10	6.84
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	10	6.84
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	10	6.84
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	10	6.84
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	10	6.84
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	11	6.84
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	11	6.84
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	11	6.84
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	11	6.84
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	11	6.84
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	11	6.84
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	10	6.84
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	10	6.84
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	10	6.84
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	10	6.84
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	10	6.84
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	10	6.84
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	11	6.84
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	11	6.84
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	11	6.84
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	11	6.84
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	11	6.84
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	11	6.84
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	10	6.84
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	10	6.84
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	10	6.84
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	10	6.84
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	10	6.84
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	10	6.84
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	11	6.84
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	11	6.84
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	11	6.84
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	11	6.84
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	11	6.84
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	11	6.84
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	3	6.8
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	3	6.8
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	3	6.8
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	3	6.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	3	6.8
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	3	6.8
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	3	6.8
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	3	6.8
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	3	6.8
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	13	6.78
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	13	6.78
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	13	6.78
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	13	6.78
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	13	6.78
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	13	6.78
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	13	6.78
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	13	6.78
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	13	6.78
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	13	6.78
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	13	6.78
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	13	6.78
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	13	6.78
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	13	6.78
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	13	6.78
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	13	6.78
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	13	6.78
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	13	6.78
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	8	6.78
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	8	6.78
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	8	6.78
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	8	6.78
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	8	6.78
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	8	6.78
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	8	6.78
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	8	6.78
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	8	6.78
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	8	6.77
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	8	6.77
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	8	6.77
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	8	6.77
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	8	6.77
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	8	6.77
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	8	6.77
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	8	6.77
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	8	6.77
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	8	6.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	8	6.77
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	8	6.77
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	8	6.77
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	8	6.77
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	8	6.77
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	8	6.77
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	8	6.77
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	8	6.77
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	10	6.76
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	10	6.76
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	10	6.76
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	10	6.76
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	10	6.76
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	10	6.76
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	10	6.76
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	10	6.76
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	10	6.76
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	7	6.73
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	7	6.73
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	7	6.73
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	7	6.73
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	7	6.73
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	7	6.73
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	7	6.73
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	7	6.73
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	7	6.73
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	14	6.72
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	14	6.72
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	14	6.72
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	14	6.72
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	14	6.72
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	14	6.72
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	14	6.72
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	14	6.72
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	14	6.72
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	14	6.72
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	14	6.72
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	14	6.72
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	14	6.72
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	14	6.72
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	14	6.72
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	14	6.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	14	6.72
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	14	6.72
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	9	6.68
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	9	6.68
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	9	6.68
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	9	6.68
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	9	6.68
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	9	6.68
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	9	6.68
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	9	6.68
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	9	6.68
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	5	6.64
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	5	6.64
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	5	6.64
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	5	6.64
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	5	6.64
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	5	6.64
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	5	6.64
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	5	6.64
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	5	6.64
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	1	6.63
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	1	6.63
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	1	6.63
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	1	6.63
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	1	6.63
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	1	6.63
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	1	6.63
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	1	6.63
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	1	6.63
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	1	6.63
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	1	6.63
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	1	6.63
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	1	6.63
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	1	6.63
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	1	6.63
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	1	6.63
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	1	6.63
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	1	6.63
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	11	6.63
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	11	6.63
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	11	6.63
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	11	6.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	11	6.63
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	11	6.63
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	2	6.59
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	2	6.59
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	2	6.59
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	2	6.59
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	2	6.59
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	2	6.59
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	2	6.59
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	2	6.59
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	2	6.59
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	9	6.58
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	9	6.58
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	9	6.58
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	9	6.58
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	9	6.58
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	9	6.58
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	9	6.58
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	9	6.58
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	9	6.58
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	9	6.58
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	9	6.58
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	9	6.58
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	9	6.58
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	9	6.58
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	9	6.58
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	9	6.58
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	9	6.58
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	9	6.58
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	3	6.58
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	3	6.58
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	10	6.58
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	10	6.58
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	3	6.58
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	3	6.58
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	10	6.58
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	10	6.58
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	3	6.58
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	3	6.58
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	10	6.58
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	10	6.58
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	4	6.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	4	6.53
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	4	6.53
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	4	6.53
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	4	6.53
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	4	6.53
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	13	6.53
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	13	6.53
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	13	6.53
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	13	6.53
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	13	6.53
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	13	6.53
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	13	6.53
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	13	6.53
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	13	6.53
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	14	6.51
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	14	6.51
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	14	6.51
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	14	6.51
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	14	6.51
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	14	6.51
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	14	6.51
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	14	6.51
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	14	6.51
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	5	6.48
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	5	6.48
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	5	6.48
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	5	6.48
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	5	6.48
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	5	6.48
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	4	6.46
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	4	6.46
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	4	6.46
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	4	6.46
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	4	6.46
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	4	6.46
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	4	6.46
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	4	6.46
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	4	6.46
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	6	6.43
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	6	6.43
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	6	6.43
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	6	6.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	6	6.43
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	6	6.43
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	6	6.43
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	6	6.43
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	6	6.43
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	6	6.38
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	6	6.38
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	6	6.38
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	6	6.38
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	6	6.38
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	6	6.38
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	6	6.38
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	6	6.38
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	6	6.38
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	6	6.38
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	6	6.38
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	6	6.38
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	6	6.38
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	6	6.38
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	6	6.38
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	6	6.38
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	6	6.38
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	6	6.38
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	14	6.38
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	14	6.38
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	14	6.38
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	14	6.38
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	14	6.38
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	14	6.38
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	9	6.36
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	9	6.36
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	9	6.36
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	9	6.36
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	9	6.36
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	9	6.36
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	6	6.27
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	6	6.27
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	6	6.27
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	6	6.27
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	6	6.27
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	6	6.27
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	12	6.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	12	6.22
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	12	6.22
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	12	6.22
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	12	6.22
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	12	6.22
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	8	6.08
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	8	6.08
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	8	6.08
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	8	6.08
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	8	6.08
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	8	6.08
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	13	6.06
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	13	6.06
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	13	6.06
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	13	6.06
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	13	6.06
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	13	6.06
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	11	5.91
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	11	5.91
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	11	5.91
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	11	5.91
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	11	5.91
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	11	5.91
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	11	5.91
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	11	5.91
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	11	5.91
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	11	5.91
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	11	5.91
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	11	5.91
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	11	5.91
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	11	5.91
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	11	5.91
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	11	5.91
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	11	5.91
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	11	5.91
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	7	5.72
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	7	5.72
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	7	5.72
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	7	5.72
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	7	5.72
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	7	5.72
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	7	5.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	7	5.72
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	7	5.72
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	7	5.72
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	7	5.72
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	7	5.72
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	7	5.72
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	7	5.72
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	7	5.72
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	7	5.72
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	7	5.72
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	7	5.72
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.69
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.69
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.69
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.69
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.69
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.69
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.69
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.69
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.69
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.69
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.69
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.69
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	15	5.69
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	15	5.69
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	15	5.69
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	15	5.69
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	15	5.69
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	15	5.69
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	12	5.66
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	12	5.66
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	12	5.66
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	12	5.66
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	12	5.66
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	12	5.66
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	12	5.66
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	12	5.66
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	12	5.66
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	12	5.66
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	12	5.66
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	12	5.66
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	12	5.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	12	5.66
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	12	5.66
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	12	5.66
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	12	5.66
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	12	5.66
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	3	5.61
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	3	5.61
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	3	5.61
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	3	5.61
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	3	5.61
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	3	5.61
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	3	5.61
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	3	5.61
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	3	5.61
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	3	5.61
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	3	5.61
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	3	5.61
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	3	5.61
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	3	5.61
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	3	5.61
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	3	5.61
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	3	5.61
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	3	5.61
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	2	5.59
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	2	5.59
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	2	5.59
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	2	5.59
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	2	5.59
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	2	5.59
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	2	5.59
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	2	5.59
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	2	5.59
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	2	5.59
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	2	5.59
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	2	5.59
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	2	5.59
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	2	5.59
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	2	5.59
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	2	5.59
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	2	5.59
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	2	5.59
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	9	5.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	9	5.53
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	9	5.53
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	9	5.53
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	9	5.53
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	9	5.53
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	9	5.53
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	9	5.53
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	9	5.53
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	9	5.53
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	9	5.53
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	9	5.53
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	9	5.53
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	9	5.53
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	9	5.53
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	9	5.53
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	9	5.53
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	9	5.53
(2,81)	1:708:A:VAL:HG21	1:714:A:PRO:HA	1	5.47
(2,81)	1:708:A:VAL:HG22	1:714:A:PRO:HA	1	5.47
(2,81)	1:708:A:VAL:HG23	1:714:A:PRO:HA	1	5.47
(2,80)	1:708:A:VAL:HG21	1:714:A:PRO:HA	1	5.47
(2,80)	1:708:A:VAL:HG22	1:714:A:PRO:HA	1	5.47
(2,80)	1:708:A:VAL:HG23	1:714:A:PRO:HA	1	5.47
(2,79)	1:708:A:VAL:HG21	1:714:A:PRO:HA	1	5.47
(2,79)	1:708:A:VAL:HG22	1:714:A:PRO:HA	1	5.47
(2,79)	1:708:A:VAL:HG23	1:714:A:PRO:HA	1	5.47
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	5	5.43
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	5	5.43
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	5	5.43
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	5	5.43
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	5	5.43
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	5	5.43
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	5	5.43
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	5	5.43
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	5	5.43
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	5	5.43
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	5	5.43
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	5	5.43
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	5	5.43
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	5	5.43
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	5	5.43
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	5	5.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	5	5.43
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	5	5.43
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	2	5.41
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	2	5.41
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	2	5.41
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	2	5.41
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	2	5.41
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	2	5.41
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	14	5.36
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	14	5.36
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	14	5.36
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	14	5.36
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	14	5.36
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	14	5.36
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	14	5.36
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	14	5.36
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	14	5.36
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	14	5.36
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	14	5.36
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	14	5.36
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	14	5.36
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	14	5.36
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	14	5.36
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	14	5.36
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	14	5.36
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	14	5.36
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	8	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	8	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	8	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	8	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	8	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	8	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	10	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	10	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	10	5.32
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	10	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	10	5.32
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	10	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	8	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	8	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	8	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	8	5.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	8	5.32
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	8	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	10	5.32
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	10	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	10	5.32
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	10	5.32
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	10	5.32
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	10	5.32
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	8	5.32
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	8	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	8	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	8	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	8	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	8	5.32
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	10	5.32
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	10	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	10	5.32
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	10	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	10	5.32
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	10	5.32
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	6	5.19
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	6	5.19
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	6	5.19
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	6	5.19
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	6	5.19
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	6	5.19
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	6	5.19
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	6	5.19
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	6	5.19
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	6	5.19
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	6	5.19
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	6	5.19
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	6	5.19
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	6	5.19
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	6	5.19
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	6	5.19
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	6	5.19
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	6	5.19
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	7	5.18
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	7	5.18
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	7	5.18
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	7	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	7	5.18
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	7	5.18
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	4	5.18
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	4	5.18
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	4	5.18
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	4	5.18
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	4	5.18
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	4	5.18
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	4	5.18
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	4	5.18
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	4	5.18
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	4	5.18
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	4	5.18
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	4	5.18
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	4	5.18
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	4	5.18
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	4	5.18
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	4	5.18
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	4	5.18
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	4	5.18
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	4	5.08
(2,99)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	4	5.08
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	4	5.08
(2,99)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	4	5.08
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	4	5.08
(2,99)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	4	5.08
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	4	5.08
(2,98)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	4	5.08
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	4	5.08
(2,98)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	4	5.08
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	4	5.08
(2,98)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	4	5.08
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE21	4	5.08
(2,97)	1:755:A:LEU:HD11	1:710:A:GLN:HE22	4	5.08
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE21	4	5.08
(2,97)	1:755:A:LEU:HD12	1:710:A:GLN:HE22	4	5.08
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE21	4	5.08
(2,97)	1:755:A:LEU:HD13	1:710:A:GLN:HE22	4	5.08
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	13	5.05
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	13	5.05
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	13	5.05
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	13	5.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	13	5.05
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	13	5.05
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	13	5.05
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	13	5.05
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	13	5.05
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	13	5.05
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	13	5.05
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	13	5.05
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	13	5.05
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	13	5.05
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	13	5.05
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	13	5.05
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	13	5.05
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	13	5.05
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	7	4.9
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	7	4.9
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	7	4.9
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	7	4.9
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	7	4.9
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	7	4.9
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	7	4.9
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	7	4.9
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	7	4.9
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	7	4.9
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	7	4.9
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	7	4.9
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	7	4.9
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	7	4.9
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	7	4.9
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	7	4.9
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	7	4.9
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	7	4.9
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD2	1	4.72
(2,84)	1:709:A:ARG:H	1:714:A:PRO:HD3	1	4.72
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD2	1	4.72
(2,83)	1:709:A:ARG:H	1:714:A:PRO:HD3	1	4.72
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD2	1	4.72
(2,82)	1:709:A:ARG:H	1:714:A:PRO:HD3	1	4.72
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	2	4.71
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	2	4.71
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	2	4.71
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	2	4.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	2	4.71
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	2	4.71
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	2	4.71
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	2	4.71
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	2	4.71
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	2	4.71
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	2	4.71
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	2	4.71
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	2	4.71
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	2	4.71
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	2	4.71
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	2	4.71
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	2	4.71
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	2	4.71
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	5	4.65
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	5	4.65
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	5	4.65
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	5	4.65
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	4.65
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	4.65
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	5	4.65
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	5	4.65
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	5	4.65
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	5	4.65
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	4.65
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	4.65
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	5	4.65
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	5	4.65
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	5	4.65
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	5	4.65
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	4.65
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	4.65
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	4.45
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	4.45
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	4.45
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	4.45
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	4.45
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	4.45
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	1	4.26
(2,78)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	1	4.26
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	1	4.26
(2,78)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	1	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	1	4.26
(2,78)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	1	4.26
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	1	4.26
(2,77)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	1	4.26
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	1	4.26
(2,77)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	1	4.26
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	1	4.26
(2,77)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	1	4.26
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD2	1	4.26
(2,76)	1:708:A:VAL:HG21	1:714:A:PRO:HD3	1	4.26
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD2	1	4.26
(2,76)	1:708:A:VAL:HG22	1:714:A:PRO:HD3	1	4.26
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD2	1	4.26
(2,76)	1:708:A:VAL:HG23	1:714:A:PRO:HD3	1	4.26
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	2	4.19
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	2	4.19
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	4.19
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	4.19
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.19
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	2	4.19
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	2	4.19
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	2	4.19
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	4.19
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	4.19
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.19
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	2	4.19
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	2	4.19
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	2	4.19
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	4.19
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	4.19
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.19
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	2	4.19
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.98
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.98
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.98
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.98
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.98
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.98
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.98
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.98
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.98
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.98
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.98
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.98
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.91
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.91
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.91
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.91
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.91
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.91
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.8
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	3.8
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	3.8
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	3.8
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	3.8
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	3.8
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.8
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	3.8
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	3.8
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	3.8
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	3.8
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	3.8
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.8
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	3.8
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	3.8
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	3.8
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	3.8
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	3.8
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.7
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.7
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.7
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.7
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.7
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.7
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.7
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.7
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	3.7
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	3.7
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.59
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.59
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.59
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.59
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.59
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.59
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.55
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.55
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.55
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.55
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.55
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.55
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.53
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.53
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.53
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.53
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.53
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.53
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.53
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.5
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.5
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	3.5
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	3.5
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.5
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.5
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	3.5
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	3.5
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.5
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.5
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	3.5
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	3.5
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.31
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.31
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.31
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.31
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.31
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.31
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	3.28
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	3.28
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	3.28
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	3.28
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	3.28
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	3.28
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	3.28
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	3.28
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	3.28
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	3.28
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	3.28
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	3.28
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	3.28
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	3.28
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	3.28
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	3.27
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	3.27
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	13	3.27
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	13	3.27
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	13	3.27
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	13	3.27
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	3.27
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	3.27
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	13	3.27
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	13	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	13	3.27
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	13	3.27
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	3.27
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	3.27
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	13	3.27
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	13	3.27
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	13	3.27
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	13	3.27
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	3.22
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	3.22
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	3.22
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	3.22
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	3.22
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	3.22
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	8	3.2
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	8	3.2
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	8	3.2
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	8	3.2
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	8	3.2
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	8	3.2
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	8	3.2
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	8	3.2
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	8	3.2
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.19
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.19
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.19
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.19
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.19
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.19
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.19
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.19
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.15
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.15
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.15
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.15
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.15
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	3.08
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	3.08
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	3.08
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.07
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.07
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.07
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.07
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.07
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.07
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.07
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.07
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.06
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.06
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.06
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.06
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.06
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	3.04
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	3.04
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	3.04
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	3.04
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	3.04
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	3.04
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	3.04
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	3.04
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	12	3.02
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	12	3.02
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	12	3.02
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	12	3.02
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	12	3.02
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	12	3.02
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	12	3.02
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	12	3.02
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	12	3.02
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.01
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.01
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.01
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.01
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.01
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.01
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.01
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.01
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.01
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.01
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.01
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.01
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	11	3.0
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	11	3.0
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	11	3.0
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	11	3.0
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	11	3.0
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	11	3.0
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	11	3.0
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	11	3.0
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	11	3.0
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	2.99
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	2.99
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	2.99
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	2.99
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	2.99
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	2.99
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	2.99
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	2.99
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	2.99
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	2.99
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	2.99
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	2.99
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	6	2.87
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	6	2.87
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	6	2.87
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	6	2.87
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	6	2.87
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	6	2.87
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	6	2.87
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	6	2.87
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	6	2.87
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	7	2.86
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	7	2.86
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	7	2.86
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	7	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	7	2.86
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	7	2.86
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	7	2.86
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	7	2.86
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	7	2.86
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	7	2.86
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	7	2.86
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	7	2.86
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	7	2.86
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	7	2.86
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	7	2.86
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	7	2.86
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	7	2.86
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	7	2.86
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	11	2.85
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	11	2.85
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	11	2.85
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	11	2.85
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	11	2.85
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	11	2.85
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	11	2.85
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	11	2.85
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	11	2.85
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	11	2.85
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	11	2.85
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	11	2.85
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	11	2.85
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	11	2.85
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	11	2.85
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	11	2.85
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	11	2.85
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	11	2.85
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	2.8
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	2.8
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	2.8
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	2.8
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	2.8
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	2.8
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	2.8
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	2.8
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	2.8
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	2.8
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	2.8
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	2.8
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.77
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.77
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.77
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.77
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.77
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.77
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	15	2.77
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	15	2.77
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	15	2.77
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	2.73
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	2.73
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	2.73
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	2.73
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	2.73
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	2.73
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	2.73
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	2.73
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.68
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.68
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.68
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.68
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.68
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.68
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.68
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.68
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.68
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.68
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.68
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	2.68
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	15	2.68
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	2.68
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	2.68
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	2.68
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	15	2.68
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	2.67
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	2.67
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	2.67
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	2.67
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	2.67
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	2.67
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	2.67
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	2.67
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	9	2.65
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	9	2.65
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	9	2.65
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	9	2.65
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	9	2.65
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	9	2.65
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	9	2.65
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	9	2.65
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	9	2.65
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	3	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	3	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	3	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	13	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	13	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	13	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	3	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	3	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	3	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	13	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	13	2.61
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	13	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	3	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	3	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	3	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	13	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	13	2.61
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	13	2.61
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	14	2.6
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	14	2.6
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	14	2.6
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	14	2.6
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	14	2.6
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	14	2.6
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	14	2.6
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	14	2.6
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	14	2.6
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.57
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.57
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.57
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.57
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.57
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.57
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.57
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.57
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.57
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.57
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.57
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.57
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.53
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.53
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.53
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.53
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.53
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.53
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.53
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.53
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.53
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.53
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.53
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.53
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.53
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.53
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.53
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.53
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.53
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.53
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.53
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.53
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.53
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.53
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.53
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.53
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.53
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.53
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	10	2.53
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	10	2.53
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	2.53
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	2.53
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	10	2.53
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	10	2.53
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	10	2.53
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	10	2.53
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	2.53
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	2.53
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	10	2.53
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	10	2.53
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	10	2.53
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	10	2.53
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	2.53
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	2.53
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	10	2.53
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	10	2.53
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.5
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.5
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.5
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.5
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.5
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	2.5
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	2.5
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	2.5
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	2.5
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	2.5
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	2.5
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	2.5
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	2.5
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	2.5
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	2.5
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.5
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.5
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.5
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	2.5
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	2.5
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	2.5
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	2.5
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	2.49
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	2.49
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	2.49
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	2.49
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	2.49
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	2.49
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.46
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.46
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.46
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.46
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.46
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.46
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.46
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.46
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.46
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.46
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.46
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.46
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.46
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.46
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.46
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.46
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.46
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.46
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.46
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.46
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.46
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.46
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.46
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.46
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.46
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.46
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.46
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.45
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.45
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.45
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.45
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.45
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.45
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	4	2.45
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	4	2.45
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	2.45
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	4	2.45
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	4	2.45
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	4	2.45
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	4	2.45
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	4	2.45
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	2.45
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	4	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	4	2.45
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	4	2.45
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	4	2.45
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	4	2.45
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	2.45
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	4	2.45
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	4	2.45
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	4	2.45
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.44
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.44
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.44
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.44
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.44
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.44
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.44
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.44
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.44
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.44
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.44
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.44
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.44
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.44
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.44
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.44
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.44
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.44
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.44
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.44
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.44
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.44
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.44
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.44
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.44
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.44
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.44
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.43
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.43
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.43
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.43
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.43
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.43
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.43
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.43
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.43
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.43
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.43
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.43
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.43
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.43
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.43
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.43
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.43
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.43
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.43
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.43
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.43
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.43
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.43
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.43
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.43
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.43
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.42
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.42
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.42
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.42
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.42
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.42
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.42
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.42
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.42
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.42
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.42
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.42
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.42
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.42
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.41
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.41
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.41
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.41
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.41
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.41
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.41
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.41
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.41
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.41
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.41
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.41
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.41
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.41
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.41
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.41
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.41
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.41
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.41
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.41
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.41
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.41
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.41
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.41
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.41
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.41
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.41
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.41
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.41
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.41
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.41
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.41
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.41
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.41
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.41
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.41
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.41
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.41
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.41
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	5	2.4
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	5	2.4
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	5	2.4
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	5	2.4
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	5	2.4
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	5	2.4
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	5	2.4
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	5	2.4
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	5	2.4
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.4
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.4
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.4
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.4
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.4
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.4
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.4
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.4
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.4
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.4
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.4
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.4
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.4
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.4
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.4
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.4
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.4
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.4
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.4
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.4
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.4
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.4
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.4
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.4
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.4
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.4
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.39
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.39
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.39
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.39
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.39
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.39
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.39
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.39
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.39
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.39
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.39
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.39
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.39
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.39
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.39
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.39
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.39
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.39
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	10	2.36
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	10	2.36
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	10	2.36
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	10	2.36
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	10	2.36
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	10	2.36
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	10	2.36
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	10	2.36
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	10	2.36
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.36
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.36
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.36
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.36
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.36
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.36
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	2.35
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	2.35
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	2.35
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	2.35
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	2.35
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	2.35
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	2.35
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	2.35
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	2.35
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	2.35
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	2.35
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	2.35
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	2.35
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	2.35
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	2.35
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	2.35
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	2.35
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	2.35
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	2.35
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	2.35
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	2.35
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	2.35
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	2.35
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	2.35
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	2.35
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	2.35
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.35
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.35
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.35
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.35
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.35
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.35
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	6	2.35
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	6	2.35
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	6	2.35
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	6	2.35
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	6	2.35
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	6	2.35
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	6	2.35
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	6	2.35
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	6	2.35
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	6	2.35
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	6	2.35
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	6	2.35
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	6	2.35
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	6	2.35
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	6	2.35
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	6	2.35
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	6	2.35
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	6	2.35
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	1	2.33
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	1	2.33
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	1	2.33
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	1	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	1	2.33
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	1	2.33
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	1	2.33
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	1	2.33
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	1	2.33
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.32
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.32
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.32
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.32
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.32
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.32
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.32
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.32
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.32
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.32
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.32
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.32
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.32
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.32
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.32
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.32
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.32
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.32
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.32
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.32
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.32
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.32
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.32
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.32
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.32
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.32
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.32
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.32
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.32
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.32
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.32
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.32
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.32
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.29
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.29
(2,66)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.29
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.29
(2,66)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.29
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.29
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.29
(2,66)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.29
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.29
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.29
(2,65)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.29
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.29
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.29
(2,65)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.29
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.29
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.29
(2,65)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.29
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.29
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.29
(2,64)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.29
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.29
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.29
(2,64)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.29
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.29
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.29
(2,64)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.29
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	2.27
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	2.27
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	1	2.27
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	1	2.27
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	1	2.27
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	1	2.27
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	2.27
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	2.27
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	1	2.27
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	1	2.27
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	1	2.27
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	1	2.27
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	2.27
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	2.27
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	1	2.27
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	1	2.27
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	1	2.27
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	1	2.27
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.26
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.26
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.26
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.26
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.26
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	5	2.21
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	5	2.21
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	5	2.21
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	5	2.21
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	5	2.21
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	5	2.21
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	5	2.21
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	5	2.21
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	5	2.21
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	5	2.21
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	5	2.21
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	5	2.21
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	5	2.21
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	5	2.21
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	5	2.21
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	5	2.21
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	5	2.21
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	5	2.21
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.21
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.21
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.21
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.21
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.21
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.21
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.21
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.21
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.21
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.21
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.21
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.21
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	1	2.2
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	1	2.2
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	1	2.2
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	1	2.2
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	1	2.2
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	1	2.2
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	1	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	1	2.2
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	1	2.2
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	1	2.2
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	1	2.2
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	1	2.2
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	1	2.2
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	1	2.2
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	1	2.2
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	1	2.2
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	1	2.2
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	1	2.2
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	3	2.16
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	3	2.16
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	3	2.16
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	3	2.16
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	3	2.16
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	3	2.16
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	4	2.16
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	4	2.16
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	4	2.16
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	4	2.16
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	4	2.16
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	4	2.16
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	3	2.16
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	3	2.16
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	3	2.16
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	3	2.16
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	3	2.16
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	3	2.16
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	4	2.16
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	4	2.16
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	4	2.16
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	4	2.16
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	4	2.16
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	4	2.16
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	3	2.16
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	3	2.16
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	3	2.16
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	3	2.16
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	3	2.16
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	3	2.16
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	4	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	4	2.16
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	4	2.16
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	4	2.16
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	4	2.16
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	4	2.16
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	7	2.15
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	7	2.15
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	7	2.15
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	7	2.15
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	7	2.15
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	7	2.15
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	7	2.15
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	7	2.15
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	7	2.15
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.15
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.15
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.15
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.15
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.15
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.15
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	14	2.14
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	14	2.14
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	14	2.14
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	14	2.14
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	14	2.14
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	14	2.14
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	14	2.14
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	14	2.14
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	14	2.14
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	14	2.14
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	14	2.14
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	14	2.14
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	14	2.14
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	14	2.14
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	14	2.14
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	14	2.14
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	14	2.14
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	14	2.14
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	2.14
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	2.14
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	9	2.14
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	9	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	9	2.14
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	9	2.14
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	2.14
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	2.14
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	9	2.14
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	9	2.14
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	9	2.14
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	9	2.14
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	2.14
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	2.14
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	9	2.14
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	9	2.14
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	9	2.14
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	9	2.14
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	11	2.09
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	11	2.09
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	11	2.09
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	11	2.09
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	11	2.09
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	11	2.09
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	11	2.09
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	11	2.09
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	11	2.09
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	11	2.09
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	11	2.09
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	11	2.09
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	11	2.09
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	11	2.09
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	11	2.09
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	11	2.09
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	11	2.09
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	11	2.09
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.09
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.09
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.09
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.09
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.09
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.09
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	4	2.08
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	4	2.08
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	4	2.08
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	4	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	4	2.08
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	4	2.08
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	4	2.08
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	4	2.08
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	4	2.08
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.08
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.08
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.08
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.08
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.08
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.08
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.08
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.08
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.08
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.08
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.08
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.08
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	15	2.08
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	15	2.08
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	15	2.08
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	15	2.08
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	15	2.08
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	15	2.08
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	8	2.08
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	8	2.08
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.08
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.08
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	2.08
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	8	2.08
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	8	2.08
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	8	2.08
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.08
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.08
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	2.08
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	8	2.08
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	8	2.08
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	8	2.08
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.08
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.08
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	2.08
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	8	2.08
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	2	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	2	2.07
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	2	2.07
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	2	2.07
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	2	2.07
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	2	2.07
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	2	2.07
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	2	2.07
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	2	2.07
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	2	2.07
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	2	2.07
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	2	2.07
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	2	2.07
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	2	2.07
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	2	2.07
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	2	2.07
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	2	2.07
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	2	2.07
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	7	2.04
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	7	2.04
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	7	2.04
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	7	2.04
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	7	2.04
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	7	2.04
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	7	2.04
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	7	2.04
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	7	2.04
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	7	2.04
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	7	2.04
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	7	2.04
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	7	2.04
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	7	2.04
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	7	2.04
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	7	2.04
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	7	2.04
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	7	2.04
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	2.01
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	2.01
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	12	2.01
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	12	2.01
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	12	2.01
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	12	2.01
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	2.01
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	12	2.01
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	12	2.01
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	12	2.01
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	12	2.01
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	2.01
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	2.01
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	12	2.01
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	12	2.01
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	12	2.01
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	12	2.01
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	3	1.99
(2,48)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	3	1.99
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	3	1.99
(2,48)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	3	1.99
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	3	1.99
(2,48)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	3	1.99
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	3	1.99
(2,47)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	3	1.99
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	3	1.99
(2,47)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	3	1.99
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	3	1.99
(2,47)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	3	1.99
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	3	1.99
(2,46)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	3	1.99
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	3	1.99
(2,46)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	3	1.99
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	3	1.99
(2,46)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	3	1.99
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.96
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.96
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.96
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.96
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.96
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.96
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	10	1.93
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	10	1.93
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	10	1.93
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	10	1.93
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	10	1.93
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	10	1.93
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	10	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	10	1.93
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	10	1.93
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	10	1.93
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	10	1.93
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	10	1.93
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	10	1.93
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	10	1.93
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	10	1.93
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	10	1.93
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	10	1.93
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	10	1.93
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	8	1.92
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	8	1.92
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	8	1.92
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	8	1.92
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	8	1.92
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	8	1.92
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	8	1.92
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	8	1.92
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	8	1.92
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	8	1.92
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	8	1.92
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	8	1.92
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	8	1.92
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	8	1.92
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	8	1.92
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	8	1.92
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	8	1.92
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	8	1.92
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.91
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.91
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.91
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.91
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.91
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.91
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	8	1.89
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	8	1.89
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	8	1.89
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	8	1.89
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	8	1.89
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	8	1.89
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	8	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	8	1.89
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	8	1.89
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	8	1.89
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	8	1.89
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	8	1.89
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	8	1.89
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	8	1.89
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	8	1.89
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	8	1.89
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	8	1.89
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	8	1.89
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	6	1.89
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	6	1.89
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	6	1.89
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	6	1.89
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	6	1.89
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	6	1.89
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	6	1.89
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	6	1.89
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	6	1.89
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	6	1.89
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	6	1.89
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	6	1.89
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	6	1.89
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	6	1.89
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	6	1.89
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	6	1.89
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	6	1.89
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	6	1.89
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	9	1.88
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	9	1.88
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	9	1.88
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	9	1.88
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	9	1.88
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	9	1.88
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	9	1.88
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	9	1.88
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	9	1.88
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	9	1.88
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	9	1.88
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	9	1.88
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	9	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	9	1.88
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	9	1.88
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	9	1.88
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	9	1.88
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	9	1.88
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.83
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.83
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.83
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.83
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.83
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.83
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.83
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.83
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.83
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.82
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.82
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.82
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.82
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.82
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.82
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.79
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.79
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.79
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.79
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.79
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.79
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	13	1.77
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	13	1.77
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	13	1.77
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	13	1.77
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	13	1.77
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	13	1.77
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	13	1.77
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	13	1.77
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	13	1.77
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	13	1.77
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	13	1.77
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	13	1.77
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	13	1.77
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	13	1.77
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	13	1.77
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	13	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	13	1.77
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	13	1.77
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	12	1.75
(2,69)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	12	1.75
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	12	1.75
(2,69)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	12	1.75
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	12	1.75
(2,69)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	12	1.75
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	12	1.75
(2,68)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	12	1.75
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	12	1.75
(2,68)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	12	1.75
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	12	1.75
(2,68)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	12	1.75
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB2	12	1.75
(2,67)	1:704:A:LEU:HD21	1:706:A:ASN:HB3	12	1.75
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB2	12	1.75
(2,67)	1:704:A:LEU:HD22	1:706:A:ASN:HB3	12	1.75
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB2	12	1.75
(2,67)	1:704:A:LEU:HD23	1:706:A:ASN:HB3	12	1.75
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	8	1.73
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	8	1.73
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	8	1.73
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.71
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.71
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.71
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.71
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.71
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.71
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.71
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.71
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.71
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.71
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.71
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.71
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.71
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.71
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.71
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.71
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.71
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.71
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	1.69
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	1.69
(2,56)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	1.69
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	1.69
(2,55)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	1.69
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.68
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.68
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.68
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.68
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.68
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.68
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.68
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.68
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.68
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.67
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.67
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.67
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.67
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.67
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.67
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.67
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.67
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.67
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.67
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.67
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.67
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.67
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.67
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.67
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.67
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.67
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.67
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.65
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.65
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.65
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.65
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.65
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.65
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.65
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.65
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.65
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.65
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.65
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.65
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.65
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.65
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.65
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.65
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.65
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.65
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.65
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.65
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.65
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.65
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.65
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.65
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.65
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.65
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.64
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.64
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.64
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.64
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.64
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.64
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.64
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.64
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.64
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.63
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.63
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.63
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.63
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.63
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.63
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.63
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.63
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.63
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.63
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.63
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.63
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.63
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.63
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.63
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.63
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.63
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.63
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.63
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.63
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.63
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.63
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.63
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.63
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.63
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.63
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	6	1.59
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	6	1.59
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	6	1.59
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG21	2	1.58
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG22	2	1.58
(2,90)	1:713:A:SER:H	1:708:A:VAL:HG23	2	1.58
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG21	2	1.58
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG22	2	1.58
(2,89)	1:713:A:SER:H	1:708:A:VAL:HG23	2	1.58
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG21	2	1.58
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG22	2	1.58
(2,88)	1:713:A:SER:H	1:708:A:VAL:HG23	2	1.58
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	8	1.53
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	8	1.53
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	8	1.53
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	13	1.51
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	13	1.51
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	13	1.51
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	4	1.5
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	4	1.5
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	4	1.5
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	6	1.49
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	6	1.49
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	6	1.49
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	8	1.48
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	8	1.48
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	8	1.48
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	10	1.46
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	14	1.46
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	8	1.46
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	10	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	14	1.46
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	8	1.46
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	10	1.46
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	14	1.46
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	8	1.46
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	5	1.43
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	5	1.43
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	5	1.43
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	3	1.43
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	3	1.43
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	3	1.43
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	5	1.41
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	6	1.41
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	5	1.41
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	6	1.41
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	5	1.41
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	6	1.41
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	11	1.4
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	11	1.4
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	11	1.4
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	8	1.39
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	8	1.39
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	8	1.39
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	15	1.37
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	15	1.37
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	15	1.37
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	4	1.34
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	4	1.34
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	4	1.34
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	8	1.32
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	8	1.32
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	8	1.32
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	9	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	9	1.31
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	9	1.31
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	4	1.3
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	8	1.3
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	4	1.3
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	8	1.3
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	4	1.3
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	8	1.3
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	2	1.29
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	2	1.29
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	2	1.29
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	1	1.28
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	11	1.28
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	14	1.28
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	6	1.28
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	7	1.28
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	1	1.28
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	11	1.28
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	14	1.28
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	6	1.28
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	7	1.28
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	1	1.28
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	11	1.28
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	14	1.28
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	6	1.28
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	7	1.28
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	10	1.26
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	13	1.26
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	9	1.26
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	4	1.26
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	10	1.26
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	13	1.26
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	9	1.26
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	4	1.26
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	10	1.26
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	13	1.26
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	9	1.26
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	4	1.26
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	7	1.25
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	7	1.25
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	7	1.25
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	7	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	7	1.25
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	7	1.25
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	7	1.25
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	7	1.25
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	7	1.25
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	7	1.25
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	7	1.25
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	7	1.25
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	7	1.25
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	7	1.25
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	7	1.25
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	7	1.25
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	7	1.25
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	7	1.25
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	1.24
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	1.24
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	1.24
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	1.24
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	1.24
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	1.24
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.23
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.23
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.23
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.23
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.23
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.23
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.23
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.23
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.23
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	11	1.23
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	11	1.23
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	11	1.23
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	7	1.22
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	13	1.22
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	7	1.22
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	13	1.22
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	7	1.22
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	13	1.22
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.21
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.21
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.21
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.21
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.21
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.21
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.21
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	3	1.21
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.21
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	5	1.21
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	3	1.21
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.21
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	5	1.21
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	3	1.21
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	15	1.21
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	5	1.21
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	6	1.2
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	13	1.2
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	6	1.2
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	13	1.2
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	6	1.2
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	13	1.2
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	6	1.19
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	1	1.19
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	6	1.19
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	1	1.19
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	6	1.19
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	1	1.19
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.18
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.18
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.18
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.18
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.18
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.18
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.18
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.18
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	12	1.18
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	5	1.18
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	12	1.18
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	5	1.18
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	12	1.18
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	5	1.18
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.17
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.17
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.17
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.17
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.17
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.17
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.17
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.17
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	12	1.17
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	11	1.17
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	12	1.17
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	11	1.17
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	12	1.17
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	11	1.17
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	6	1.16
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	6	1.16
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	6	1.16
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	6	1.16
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	6	1.16
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	6	1.16
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	6	1.16
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	6	1.16
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	6	1.16
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	6	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	6	1.16
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	6	1.16
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	6	1.16
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	6	1.16
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	6	1.16
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	6	1.16
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	6	1.16
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	6	1.16
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.15
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.15
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.15
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.14
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.14
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.14
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.14
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.14
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.14
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.14
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.14
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	4	1.14
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	4	1.14
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	4	1.14
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.13
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.13
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.13
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.13
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	14	1.13
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	10	1.13
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	14	1.13
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	10	1.13
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	14	1.13
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	10	1.13
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	11	1.12
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	13	1.12
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	14	1.12
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	11	1.12
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	11	1.12
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	13	1.12
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	14	1.12
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	10	1.12
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	11	1.12
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	11	1.12
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	13	1.12
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	14	1.12
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	10	1.12
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	11	1.12
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	1.11
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	1.11
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	1.11
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	1.11
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	1.11
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	1.11
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	3	1.11
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	11	1.11
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	3	1.11
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	11	1.11
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	3	1.11
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	11	1.11
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	9	1.1
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	2	1.1
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	9	1.1
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	2	1.1
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	9	1.1
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	2	1.1
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	2	1.09
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	10	1.09
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	2	1.09
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	10	1.09
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	2	1.09
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	10	1.09
(2,39)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.08
(2,39)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.08
(2,39)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.08
(2,38)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.08
(2,38)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.08
(2,38)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.08
(2,37)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.08
(2,37)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.08
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	1	1.08
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	11	1.08
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	1	1.08
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	11	1.08
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	1	1.08
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	11	1.08
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	14	1.07
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	14	1.07
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	14	1.07
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	7	1.06
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	9	1.06
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	7	1.06
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	9	1.06
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	7	1.06
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	9	1.06
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.05
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	15	1.05
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.05
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	15	1.05
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	15	1.05
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	15	1.05
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	3	1.04
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	9	1.04
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	3	1.04
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	9	1.04
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	3	1.04
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	9	1.04
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	4	1.03
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	10	1.03
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	4	1.03
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	10	1.03
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	4	1.03
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	10	1.03
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	3	1.02
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	4	1.02
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	3	1.02
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	4	1.02
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	3	1.02
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	4	1.02
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	1.01
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	1.01
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	1.01
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	1.01
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	1.01
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	6	1.01
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	1	1.01
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	6	1.01
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	1	1.01
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	6	1.01
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	1	1.01
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	4	1.0
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	4	1.0
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	4	1.0
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	12	0.99
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	12	0.99
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	12	0.99
(2,1080)	1:697:A:ILE:HG21	1:698:A:VAL:HA	15	0.98
(2,1080)	1:697:A:ILE:HG22	1:698:A:VAL:HA	15	0.98
(2,1080)	1:697:A:ILE:HG23	1:698:A:VAL:HA	15	0.98
(2,674)	1:697:A:ILE:HG21	1:698:A:VAL:HA	15	0.98
(2,674)	1:697:A:ILE:HG22	1:698:A:VAL:HA	15	0.98
(2,674)	1:697:A:ILE:HG23	1:698:A:VAL:HA	15	0.98
(2,268)	1:697:A:ILE:HG21	1:698:A:VAL:HA	15	0.98
(2,268)	1:697:A:ILE:HG22	1:698:A:VAL:HA	15	0.98
(2,268)	1:697:A:ILE:HG23	1:698:A:VAL:HA	15	0.98
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	12	0.96
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	12	0.96
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	12	0.96
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	12	0.96
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	12	0.96
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	12	0.96
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	12	0.96
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	12	0.96
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	12	0.96
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	12	0.96
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	12	0.96
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	12	0.96
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	12	0.96
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	12	0.96
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	12	0.96
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	12	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	12	0.96
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	12	0.96
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	4	0.96
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	4	0.96
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	4	0.96
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	6	0.95
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	6	0.95
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	6	0.95
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	13	0.94
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	13	0.94
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	13	0.94
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	13	0.94
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	13	0.94
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	13	0.94
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	13	0.94
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	13	0.94
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	13	0.94
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	13	0.94
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	13	0.94
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	13	0.94
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	13	0.94
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	13	0.94
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	13	0.94
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	13	0.94
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	13	0.94
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	13	0.94
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	1	0.94
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	15	0.94
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	1	0.94
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	15	0.94
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	1	0.94
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	15	0.94
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	9	0.93
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	7	0.93
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	9	0.93
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	7	0.93
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	9	0.93
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	7	0.93
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	7	0.92
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	10	0.92
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	7	0.92
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	10	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	7	0.92
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	10	0.92
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	13	0.91
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	13	0.91
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	13	0.91
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	5	0.9
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	5	0.9
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	5	0.9
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	1	0.89
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	8	0.89
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	1	0.89
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	8	0.89
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	1	0.89
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	8	0.89
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	14	0.88
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	14	0.88
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	14	0.88
(1,65)	1:746:C:ILE:O	1:750:C:ASN:H	5	0.87
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	13	0.87
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	13	0.87
(1,39)	1:746:C:ILE:O	1:750:C:ASN:H	5	0.87
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	13	0.87
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	13	0.87
(1,13)	1:746:C:ILE:O	1:750:C:ASN:H	5	0.87
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	13	0.87
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	13	0.87
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	14	0.86
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	14	0.86
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	14	0.86
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	11	0.86
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	11	0.86
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	11	0.86
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	14	0.85
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	14	0.85
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	14	0.85
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	10	0.84
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	10	0.84
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	10	0.84
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	11	0.83
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	12	0.83
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	13	0.83
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	5	0.83
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	11	0.83
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	12	0.83
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	13	0.83
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	3	0.83
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	5	0.83
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	11	0.83
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	12	0.83
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	13	0.83
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	3	0.83
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	5	0.83
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	8	0.82
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	8	0.82
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	8	0.82
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	3	0.82
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	3	0.82
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	3	0.82
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	12	0.81
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	12	0.81
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	12	0.81
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	14	0.81
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	12	0.81
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	7	0.81
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	14	0.81
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	12	0.81
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	7	0.81
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	14	0.81
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	12	0.81
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	7	0.81
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.8
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	7	0.8
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.8
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	7	0.8
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	7	0.8
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	7	0.8
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	1	0.8
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	11	0.8
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	1	0.8
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	11	0.8
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	1	0.8
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	11	0.8
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	1	0.79
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	1	0.79
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	9	0.79
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	9	0.79
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	9	0.79
(2,1016)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.78
(2,1016)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.78
(2,1016)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.78
(2,1016)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.78
(2,1016)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.78
(2,1016)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.78
(2,610)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.78
(2,204)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.78
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	13	0.78
(1,66)	1:746:C:ILE:O	1:750:C:ASN:N	5	0.78
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	13	0.78
(1,40)	1:746:C:ILE:O	1:750:C:ASN:N	5	0.78
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	13	0.78
(1,14)	1:746:C:ILE:O	1:750:C:ASN:N	5	0.78
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	0.77
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	0.77
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	0.77
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	0.77
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	0.77
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	0.77
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	3	0.77
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	11	0.77
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	12	0.77
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	6	0.77
(1,63)	1:745:C:SER:O	1:749:C:VAL:H	5	0.77
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	2	0.77
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	3	0.77
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	3	0.77
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	11	0.77
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	12	0.77
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	6	0.77
(1,37)	1:745:C:SER:O	1:749:C:VAL:H	5	0.77
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	2	0.77
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	10	0.77
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	3	0.77
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	3	0.77
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	11	0.77
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	12	0.77
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	6	0.77
(1,11)	1:745:C:SER:O	1:749:C:VAL:H	5	0.77
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	2	0.77
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	10	0.77
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	3	0.77
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	11	0.76
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	11	0.76
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	11	0.76
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	15	0.76
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	15	0.76
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	15	0.76
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	15	0.76
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	15	0.76
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	15	0.76
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	15	0.76
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	15	0.76
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	15	0.76
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	15	0.76
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	15	0.76
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	15	0.76
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	15	0.76
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	15	0.76
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	15	0.76
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	15	0.76
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	15	0.76
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	15	0.76
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	1	0.76
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	1	0.76
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	1	0.76
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.75
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.75
(2,41)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.75
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.75
(2,40)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.75
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	2	0.74
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	1	0.74
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	14	0.74
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	3	0.74
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	2	0.74
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	1	0.74
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	14	0.74
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	3	0.74
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	2	0.74
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	1	0.74
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	14	0.74
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	3	0.74
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	10	0.73
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	10	0.73
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	10	0.73
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.73
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.73
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.73
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.73
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.73
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.73
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.73
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.73
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.73
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	9	0.73
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	13	0.73
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	9	0.73
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	13	0.73
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	9	0.73
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	13	0.73
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.72
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.72
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.72
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.72
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.72
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.72
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.72
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.72
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.72
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.72
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.72
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.72
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.72
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.72
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.72
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.72
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.72
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	0.72
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	0.72
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	0.72
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	0.72
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	0.72
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	0.72
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	0.72
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	0.72
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	0.72
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	3	0.72
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.72
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	3	0.72
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.72
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	3	0.72
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	15	0.72
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	11	0.71
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	11	0.71
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	11	0.71
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	11	0.71
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	11	0.71
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	11	0.71
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	11	0.71
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	11	0.71
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	11	0.71
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	11	0.71
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	11	0.71
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	11	0.71
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	11	0.71
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	11	0.71
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	11	0.71
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	11	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	11	0.71
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	11	0.71
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	4	0.71
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	4	0.71
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	4	0.71
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	12	0.7
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	12	0.7
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	12	0.7
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	12	0.7
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	12	0.7
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	12	0.7
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	6	0.7
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	8	0.7
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	5	0.7
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	6	0.7
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	8	0.7
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	5	0.7
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	6	0.7
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	8	0.7
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	5	0.7
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	13	0.69
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	13	0.69
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD2	13	0.69
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	14	0.68
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	14	0.68
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	8	0.68
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	14	0.68
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	14	0.68
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	8	0.68
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	14	0.68
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	14	0.68
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	8	0.68
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	7	0.68
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	7	0.68
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	7	0.68
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	10	0.67
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	10	0.67
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	10	0.67
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	4	0.67
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	4	0.67
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	4	0.67
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	4	0.67
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	4	0.67
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	4	0.67
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	4	0.67
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	4	0.67
(2,1244)	1:759:A:ASP:H	1:759:A:ASP:HB2	3	0.66
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	6	0.66
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	3	0.66
(2,838)	1:759:A:ASP:H	1:759:A:ASP:HB2	3	0.66
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	6	0.66
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	3	0.66
(2,432)	1:759:A:ASP:H	1:759:A:ASP:HB2	3	0.66
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	6	0.66
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	3	0.66
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	4	0.65
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	4	0.65
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	4	0.65
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.65
(1,61)	1:744:C:ARG:O	1:748:C:LEU:H	12	0.65
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.65
(1,35)	1:744:C:ARG:O	1:748:C:LEU:H	12	0.65
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	15	0.65
(1,9)	1:744:C:ARG:O	1:748:C:LEU:H	12	0.65
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	13	0.64
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	13	0.64
(2,1172)	1:710:A:GLN:H	1:710:A:GLN:HB2	15	0.64
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	13	0.64
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	13	0.64
(2,766)	1:710:A:GLN:H	1:710:A:GLN:HB2	15	0.64
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	13	0.64
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	13	0.64
(2,360)	1:710:A:GLN:H	1:710:A:GLN:HB2	15	0.64
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.64
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.64
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.64
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.64
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.64
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.64
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.64
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.64
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.64
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.64
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.64
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	14	0.64
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	14	0.64
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	14	0.64
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	14	0.64
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	14	0.64
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	14	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.64
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.64
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.64
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	0.64
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	0.64
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	0.64
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.64
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.64
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.64
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.64
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.64
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.64
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.64
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.64
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.63
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.63
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	15	0.63
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	2	0.62
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	2	0.62
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	6	0.62
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	6	0.62
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.62
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.62
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	10	0.62
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	10	0.62
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	10	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	2	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	2	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	6	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	6	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.62
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.62
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	10	0.62
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	10	0.62
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	10	0.62
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	2	0.62
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	6	0.62
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	6	0.62
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	15	0.62
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	15	0.62
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	10	0.62
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	10	0.62
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	10	0.62
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	2	0.62
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	2	0.62
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	2	0.62
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	2	0.62
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	2	0.62
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	2	0.62
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	2	0.62
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	2	0.62
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	2	0.62
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	2	0.62
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	2	0.62
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	2	0.62
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	2	0.62
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	2	0.62
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	2	0.62
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	2	0.62
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	2	0.62
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	2	0.62
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.62
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.62
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.62
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.62
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.62
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.62
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.62
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.62
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.62
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.62
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.62
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.62
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.62
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.62
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.62
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.62
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.62
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.62
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.62
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.62
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.62
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.62
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.62
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.62
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.62
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.62
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	7	0.62
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	7	0.62
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	7	0.62
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	6	0.61
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	6	0.61
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	6	0.61
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	4	0.61
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	4	0.61
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	4	0.61
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	9	0.6
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	9	0.6
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	12	0.6
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	12	0.6
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	14	0.6
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	14	0.6
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	14	0.6
(2,1172)	1:710:A:GLN:H	1:710:A:GLN:HB2	6	0.6
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.6
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.6
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.6
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.6
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	9	0.6
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	9	0.6
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	12	0.6
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	12	0.6
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	14	0.6
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	14	0.6
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	14	0.6
(2,766)	1:710:A:GLN:H	1:710:A:GLN:HB2	6	0.6
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.6
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.6
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.6
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	9	0.6
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	9	0.6
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	12	0.6
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	12	0.6
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	14	0.6
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	14	0.6
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	14	0.6
(2,360)	1:710:A:GLN:H	1:710:A:GLN:HB2	6	0.6
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.6
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.6
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.6
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	15	0.6
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	9	0.59
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.59
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.59
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.59
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.59
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	9	0.59
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.59
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.59
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.59
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.59
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	9	0.59
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	15	0.59
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	15	0.59
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	15	0.59
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.59
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.59
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.59
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.59
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.59
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.59
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.59
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.59
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.59
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.59
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.59
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.59
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.59
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.59
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	10	0.58
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	10	0.58
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	10	0.58
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	10	0.58
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	10	0.58
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.58
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.58
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.58
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.58
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.58
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.58
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.58
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.58
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.58
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.58
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.58
(2,51)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.58
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.58
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.58
(2,50)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.58
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.58
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.58
(2,49)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.58
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.58
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.58
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.58
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.58
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.58
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.58
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	12	0.58
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	12	0.58
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	12	0.58
(2,1243)	1:759:A:ASP:H	1:759:A:ASP:HB3	15	0.57
(2,837)	1:759:A:ASP:H	1:759:A:ASP:HB3	15	0.57
(2,431)	1:759:A:ASP:H	1:759:A:ASP:HB3	15	0.57
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.57
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.57
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.57
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.57
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.57
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.57
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.57
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.57
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.57
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.57
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.57
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.57
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.57
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.57
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.57
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.57
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.57
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.57
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.57
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.57
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.57
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.57
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.57
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.57
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.57
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.57
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	10	0.57
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	13	0.57
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	10	0.57
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	13	0.57
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	10	0.57
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	13	0.57
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	1	0.56
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	1	0.56
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	1	0.56
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	12	0.56
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	12	0.56
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	12	0.56
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	15	0.56
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	5	0.56
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	5	0.56
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.56
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	1	0.56
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	1	0.56
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	1	0.56
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	12	0.56
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	12	0.56
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	12	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	15	0.56
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	5	0.56
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	5	0.56
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.56
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	1	0.56
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	1	0.56
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	1	0.56
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	12	0.56
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	12	0.56
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	12	0.56
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	15	0.56
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	5	0.56
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	5	0.56
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.56
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	9	0.56
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	9	0.56
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	9	0.56
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	9	0.56
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	9	0.56
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	9	0.56
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	13	0.55
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	13	0.55
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	13	0.55
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.55
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.55
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.55
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	15	0.55
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	15	0.55
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	15	0.55
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	13	0.55
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	13	0.55
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	13	0.55
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.55
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.55
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.55
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	15	0.55
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	15	0.55
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	15	0.55
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	13	0.55
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	13	0.55
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	13	0.55
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.55
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.55
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	15	0.55
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	15	0.55
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	15	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.55
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.55
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.55
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.55
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.55
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.55
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.55
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.55
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.55
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.55
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.55
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.55
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.55
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.55
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	13	0.55
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	13	0.55
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	13	0.55
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	13	0.55
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	13	0.55
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	13	0.55
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.55
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.55
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	15	0.55
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	3	0.54
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	3	0.54
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.54
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.54
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	14	0.54
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	14	0.54
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	14	0.54
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	3	0.54
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	3	0.54
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	3	0.54
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.54
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.54
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	14	0.54
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	14	0.54
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	14	0.54
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	3	0.54
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	3	0.54
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	3	0.54
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.54
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.54
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	14	0.54
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	14	0.54
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	14	0.54
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.54
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.54
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.54
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.54
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.54
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.54
(1,64)	1:745:C:SER:O	1:749:C:VAL:N	5	0.54
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	14	0.54
(1,38)	1:745:C:SER:O	1:749:C:VAL:N	5	0.54
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	14	0.54
(1,12)	1:745:C:SER:O	1:749:C:VAL:N	5	0.54
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	14	0.54
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	4	0.53
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	13	0.53
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.53
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.53
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	4	0.53
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	13	0.53
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.53
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	4	0.53
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	13	0.53
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.53
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.53
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.53
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.53
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.53
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.53
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.53
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.53
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.53
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.53
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.53
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.53
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.53
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.53
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	8	0.53
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	8	0.53
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	8	0.53
(2,1347)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	7	0.52
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	8	0.52
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	7	0.52
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	3	0.52
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	4	0.52
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.52
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.52
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.52
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.52
(2,941)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	7	0.52
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	8	0.52
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	7	0.52
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	3	0.52
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	4	0.52
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.52
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.52
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.52
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.52
(2,535)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	7	0.52
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	8	0.52
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	7	0.52
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	4	0.52
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.52
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.52
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.52
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.52
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.52
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.52
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.52
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.52
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.52
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.52
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.52
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.52
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.52
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.52
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.52
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.52
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.52
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.52
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.52
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.52
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.52
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.52
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.52
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.52
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.52
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.52
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.52
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.52
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.52
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.52
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.52
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	10	0.52
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	2	0.52
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	10	0.52
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	2	0.52
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	10	0.52
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	2	0.52
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	10	0.51
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	1	0.51
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	1	0.51
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	10	0.51
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	1	0.51
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	1	0.51
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	4	0.51
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	10	0.51
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	1	0.51
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	1	0.51
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	4	0.51
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.51
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.51
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.51
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.51
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.51
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.51
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.51
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.51
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.51
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.51
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.51
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.51
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.51
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.51
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.51
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.51
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.51
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.51
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.51
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.51
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.51
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.51
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.51
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.51
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.51
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.51
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.51
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	7	0.51
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	7	0.51
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	7	0.51
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	1	0.5
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	9	0.5
(2,1347)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	15	0.5
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	2	0.5
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	2	0.5
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	2	0.5
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.5
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.5
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.5
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	1	0.5
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	9	0.5
(2,941)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	15	0.5
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	5	0.5
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	2	0.5
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	2	0.5
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	2	0.5
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.5
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.5
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.5
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	1	0.5
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	9	0.5
(2,535)	1:780:A:ARG:HH21	1:783:A:GLU:OE1	15	0.5
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	5	0.5
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	2	0.5
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	2	0.5
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	2	0.5
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.5
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.5
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.5
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	10	0.5
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	10	0.5
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	10	0.5
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	10	0.5
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	10	0.5
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	10	0.5
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	10	0.5
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	10	0.5
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	10	0.5
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	10	0.5
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	10	0.5
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	10	0.5
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	10	0.5
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	10	0.5
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	10	0.5
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	10	0.5
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	10	0.5
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	3	0.5
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	3	0.5
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	3	0.5
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	3	0.5
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	3	0.5
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	3	0.5
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	1	0.5
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	6	0.5
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	9	0.5
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	1	0.5
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	6	0.5
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	9	0.5
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	1	0.5
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	6	0.5
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	9	0.5
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	11	0.49
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	11	0.49
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	11	0.49
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	7	0.49
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.49
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.49
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.49
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.49
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.49
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.49
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	11	0.49
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	11	0.49
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	11	0.49
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	7	0.49
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.49
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.49
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.49
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.49
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.49
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.49
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	11	0.49
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	11	0.49
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	11	0.49
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	7	0.49
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.49
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.49
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.49
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.49
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.49
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	12	0.49
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	12	0.49
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	12	0.49
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	2	0.48
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	4	0.48
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	4	0.48
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	14	0.48
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	14	0.48
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.48
(2,1061)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	6	0.48
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	2	0.48
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	4	0.48
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	4	0.48
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	14	0.48
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	14	0.48
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.48
(2,655)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	6	0.48
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	2	0.48
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	4	0.48
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	4	0.48
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	14	0.48
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	14	0.48
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.48
(2,249)	1:692:A:LEU:HD13	1:696:A:ARG:HH22	6	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.48
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.48
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.48
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.48
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.48
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.48
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.48
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.48
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.48
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.48
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.48
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.48
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.48
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.48
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	6	0.47
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	9	0.47
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	9	0.47
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	9	0.47
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	14	0.47
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.47
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.47
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.47
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.47
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.47
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.47
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	6	0.47
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	6	0.47
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	9	0.47
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	9	0.47
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	9	0.47
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	14	0.47
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.47
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.47
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.47
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.47
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.47
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.47
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	6	0.47
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	6	0.47
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	9	0.47
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	9	0.47
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	9	0.47
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	14	0.47
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.47
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.47
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.47
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.47
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.47
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.47
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.47
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.47
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.47
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.47
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.47
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.47
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.47
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.47
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.47
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.47
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.47
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.47
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.47
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.47
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.47
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.47
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.47
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.47
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.47
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.47
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.47
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.47
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.47
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.47
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.47
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.47
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	1	0.47
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	1	0.47
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	1	0.47
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	11	0.46
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	7	0.46
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	8	0.46
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.46
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.46
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	11	0.46
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	7	0.46
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	8	0.46
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.46
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.46
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	11	0.46
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	7	0.46
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	8	0.46
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.46
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.46
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	9	0.46
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	9	0.46
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	9	0.46
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	9	0.46
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	9	0.46
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	14	0.45
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	3	0.45
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.45
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.45
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.45
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.45
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.45
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	8	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	8	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	8	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	8	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	8	0.45
(2,1013)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	8	0.45
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	14	0.45
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	3	0.45
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.45
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.45
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.45
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.45
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.45
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	8	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	8	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	8	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	8	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	8	0.45
(2,607)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	8	0.45
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	14	0.45
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	3	0.45
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	15	0.45
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	15	0.45
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	15	0.45
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	15	0.45
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	15	0.45
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	15	0.45
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	8	0.45
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	8	0.45
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	8	0.45
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	8	0.45
(2,201)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	8	0.45
(2,1346)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	1	0.44
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	12	0.44
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	5	0.44
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	5	0.44
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	14	0.44
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	14	0.44
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	14	0.44
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.44
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.44
(2,1061)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	9	0.44
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.44
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.44
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.44
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.44
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.44
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.44
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.44
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.44
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.44
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.44
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.44
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.44
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.44
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.44
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.44
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.44
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.44
(2,940)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	1	0.44
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	12	0.44
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	5	0.44
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	5	0.44
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	14	0.44
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	14	0.44
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	14	0.44
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.44
(2,655)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	9	0.44
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.44
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.44
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.44
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.44
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.44
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.44
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.44
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.44
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.44
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.44
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.44
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.44
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.44
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.44
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.44
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.44
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.44
(2,534)	1:770:A:ARG:HH12	1:773:A:ASP:OD1	1	0.44
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	12	0.44
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	5	0.44
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	5	0.44
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	14	0.44
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	14	0.44
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	14	0.44
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.44
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.44
(2,249)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	9	0.44
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.44
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.44
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.44
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.44
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.44
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.44
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.44
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.44
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.44
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.44
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.44
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.44
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.44
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.44
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.44
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.44
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	1	0.44
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	1	0.44
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	1	0.44
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	1	0.44
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	1	0.44
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	1	0.44
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	1	0.44
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	1	0.44
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	1	0.44
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	1	0.44
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	1	0.44
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	1	0.44
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	1	0.44
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	1	0.44
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	1	0.44
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	1	0.44
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	1	0.44
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	1	0.44
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	7	0.44
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	8	0.44
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	7	0.44
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	8	0.44
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	7	0.44
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	8	0.44
(2,1344)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	14	0.43
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	12	0.43
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	1	0.43
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	3	0.43
(2,1131)	1:705:A:VAL:HG21	1:701:A:VAL:HA	8	0.43
(2,1131)	1:705:A:VAL:HG22	1:701:A:VAL:HA	8	0.43
(2,1131)	1:705:A:VAL:HG23	1:701:A:VAL:HA	8	0.43
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.43
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.43
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.43
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.43
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.43
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.43
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.43
(2,938)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	14	0.43
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	12	0.43
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	1	0.43
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	11	0.43
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	3	0.43
(2,725)	1:705:A:VAL:HG21	1:701:A:VAL:HA	8	0.43
(2,725)	1:705:A:VAL:HG22	1:701:A:VAL:HA	8	0.43
(2,725)	1:705:A:VAL:HG23	1:701:A:VAL:HA	8	0.43
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.43
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.43
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.43
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.43
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.43
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.43
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.43
(2,532)	1:744:A:ARG:HH22	1:741:A:ASP:OD1	14	0.43
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	12	0.43
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	1	0.43
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	11	0.43
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	3	0.43
(2,319)	1:705:A:VAL:HG21	1:701:A:VAL:HA	8	0.43
(2,319)	1:705:A:VAL:HG22	1:701:A:VAL:HA	8	0.43
(2,319)	1:705:A:VAL:HG23	1:701:A:VAL:HA	8	0.43
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.43
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.43
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.43
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.43
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.43
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.43
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.43
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.43
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.43
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.43
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.43
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.43
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.43
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.43
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.43
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.43
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.43
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.43
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.43
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.43
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.43
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.43
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.43
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.43
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.43
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.43
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.43
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.43
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.43
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.43
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.43
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.43
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.43
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	2	0.43
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	7	0.43
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	1	0.43
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	2	0.43
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	7	0.43
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	1	0.43
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	2	0.43
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	7	0.43
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	1	0.43
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	6	0.42
(2,1343)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	7	0.42
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	10	0.42
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	2	0.42
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.42
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.42
(2,1131)	1:705:A:VAL:HG21	1:701:A:VAL:HA	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1131)	1:705:A:VAL:HG22	1:701:A:VAL:HA	15	0.42
(2,1131)	1:705:A:VAL:HG23	1:701:A:VAL:HA	15	0.42
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	6	0.42
(2,937)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	7	0.42
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	10	0.42
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	2	0.42
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.42
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.42
(2,725)	1:705:A:VAL:HG21	1:701:A:VAL:HA	15	0.42
(2,725)	1:705:A:VAL:HG22	1:701:A:VAL:HA	15	0.42
(2,725)	1:705:A:VAL:HG23	1:701:A:VAL:HA	15	0.42
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD1	6	0.42
(2,531)	1:740:A:ARG:HH21	1:743:A:ASP:OD1	7	0.42
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	10	0.42
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	2	0.42
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.42
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.42
(2,319)	1:705:A:VAL:HG21	1:701:A:VAL:HA	15	0.42
(2,319)	1:705:A:VAL:HG22	1:701:A:VAL:HA	15	0.42
(2,319)	1:705:A:VAL:HG23	1:701:A:VAL:HA	15	0.42
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	3	0.42
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	3	0.42
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	3	0.42
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	1	0.41
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	14	0.41
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	12	0.41
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	11	0.41
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	11	0.41
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	7	0.41
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	7	0.41
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	7	0.41
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	8	0.41
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	8	0.41
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	8	0.41
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	5	0.41
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.41
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.41
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.41
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	1	0.41
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	14	0.41
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	12	0.41
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	11	0.41
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	7	0.41
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	7	0.41
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	7	0.41
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	8	0.41
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	8	0.41
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	8	0.41
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	5	0.41
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.41
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.41
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.41
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	1	0.41
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	14	0.41
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	12	0.41
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	11	0.41
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	11	0.41
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	7	0.41
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	7	0.41
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	7	0.41
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	8	0.41
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	8	0.41
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	8	0.41
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	5	0.41
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.41
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.41
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.41
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	9	0.41
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	9	0.41
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	9	0.41
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	9	0.41
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	9	0.41
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	9	0.41
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	9	0.41
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	9	0.41
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	9	0.41
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	9	0.41
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	9	0.41
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	9	0.41
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	9	0.41
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	9	0.41
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	9	0.41
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	9	0.41
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	9	0.41
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	12	0.41
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	12	0.41
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	12	0.41
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	12	0.41
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	12	0.41
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	12	0.41
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	8	0.41
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	9	0.41
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	2	0.41
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.41
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	12	0.41
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	2	0.41
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	6	0.41
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	8	0.41
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	9	0.41
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	2	0.41
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.41
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	12	0.41
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	2	0.41
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	6	0.41
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	8	0.41
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	9	0.41
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	2	0.41
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	15	0.41
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	12	0.41
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	2	0.41
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	6	0.41
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	11	0.4
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	2	0.4
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	4	0.4
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	7	0.4
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	7	0.4
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	12	0.4
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	15	0.4
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	10	0.4
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	10	0.4
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	10	0.4
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	3	0.4
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	12	0.4
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.4
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.4
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.4
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.4
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.4
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	11	0.4
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	2	0.4
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	4	0.4
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	7	0.4
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	7	0.4
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	12	0.4
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	15	0.4
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	10	0.4
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	10	0.4
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	10	0.4
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	3	0.4
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	12	0.4
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.4
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.4
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.4
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.4
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.4
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.4
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	11	0.4
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	2	0.4
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	4	0.4
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	7	0.4
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	7	0.4
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	12	0.4
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	15	0.4
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	10	0.4
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	10	0.4
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	10	0.4
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	3	0.4
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	12	0.4
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.4
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.4
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.4
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.4
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.4
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.4
(2,1343)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	5	0.39
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	5	0.39
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	10	0.39
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.39
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	6	0.39
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	6	0.39
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	6	0.39
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	13	0.39
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	13	0.39
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	13	0.39
(2,1171)	1:710:A:GLN:H	1:710:A:GLN:HB3	10	0.39
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	6	0.39
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	6	0.39
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	6	0.39
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	6	0.39
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	6	0.39
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	6	0.39
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	13	0.39
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	13	0.39
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	13	0.39
(2,1129)	1:705:A:VAL:HG11	1:706:A:ASN:HA	8	0.39
(2,1129)	1:705:A:VAL:HG12	1:706:A:ASN:HA	8	0.39
(2,1129)	1:705:A:VAL:HG13	1:706:A:ASN:HA	8	0.39
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.39
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.39
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.39
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	6	0.39
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	2	0.39
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	15	0.39
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	15	0.39
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	15	0.39
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	15	0.39
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	15	0.39
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	15	0.39
(2,937)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	14	0.39
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	5	0.39
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	5	0.39
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	10	0.39
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.39
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	6	0.39
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	6	0.39
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	13	0.39
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	13	0.39
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	13	0.39
(2,765)	1:710:A:GLN:H	1:710:A:GLN:HB3	10	0.39
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	6	0.39
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	6	0.39
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	6	0.39
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	6	0.39
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	6	0.39
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	6	0.39
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	13	0.39
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	13	0.39
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	13	0.39
(2,723)	1:705:A:VAL:HG11	1:706:A:ASN:HA	8	0.39
(2,723)	1:705:A:VAL:HG12	1:706:A:ASN:HA	8	0.39
(2,723)	1:705:A:VAL:HG13	1:706:A:ASN:HA	8	0.39
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.39
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.39
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.39
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	6	0.39
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	2	0.39
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	15	0.39
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	15	0.39
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	15	0.39
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	15	0.39
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	15	0.39
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	15	0.39
(2,531)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	14	0.39
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	5	0.39
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	5	0.39
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	10	0.39
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	15	0.39
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	6	0.39
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	6	0.39
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	6	0.39
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	13	0.39
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	13	0.39
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	13	0.39
(2,359)	1:710:A:GLN:H	1:710:A:GLN:HB3	10	0.39
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	6	0.39
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	6	0.39
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	6	0.39
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	6	0.39
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	6	0.39
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	13	0.39
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	13	0.39
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	13	0.39
(2,317)	1:705:A:VAL:HG11	1:706:A:ASN:HA	8	0.39
(2,317)	1:705:A:VAL:HG12	1:706:A:ASN:HA	8	0.39
(2,317)	1:705:A:VAL:HG13	1:706:A:ASN:HA	8	0.39
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.39
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.39
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.39
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	6	0.39
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	2	0.39
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	15	0.39
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	15	0.39
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	15	0.39
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	15	0.39
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	15	0.39
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	15	0.39
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	5	0.39
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	5	0.39
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	5	0.39
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	5	0.39
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	5	0.39
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	5	0.39
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	10	0.39
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	10	0.39
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	10	0.39
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	3	0.38
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	11	0.38
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	2	0.38
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	1	0.38
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	4	0.38
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	4	0.38
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	4	0.38
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.38
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.38
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.38
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	11	0.38
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.38
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.38
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.38
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.38
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.38
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.38
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.38
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.38
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.38
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.38
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.38
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.38
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.38
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.38
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.38
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.38
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.38
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	3	0.38
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	11	0.38
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	2	0.38
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	1	0.38
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	4	0.38
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	4	0.38
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	4	0.38
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.38
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.38
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.38
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	11	0.38
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.38
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.38
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.38
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.38
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.38
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.38
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.38
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.38
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.38
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.38
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.38
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.38
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.38
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.38
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.38
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.38
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.38
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	3	0.38
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	11	0.38
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	2	0.38
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	1	0.38
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	4	0.38
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	4	0.38
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	4	0.38
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	15	0.38
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	15	0.38
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	15	0.38
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	11	0.38
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.38
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.38
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.38
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.38
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.38
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.38
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.38
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.38
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.38
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.38
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.38
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.38
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.38
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.38
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.38
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.38
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.38
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.38
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.38
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.38
(2,33)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.38
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.38
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.38
(2,33)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.38
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.38
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.38
(2,33)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.38
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.38
(2,32)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.38
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.38
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.38
(2,32)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.38
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.38
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.38
(2,32)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.38
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.38
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.38
(2,31)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.38
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.38
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.38
(2,31)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.38
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.38
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.38
(2,31)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.38
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	7	0.38
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	7	0.38
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	7	0.38
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	4	0.37
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	4	0.37
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	6	0.37
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	10	0.37
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	1	0.37
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	1	0.37
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	1	0.37
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	12	0.37
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	12	0.37
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	12	0.37
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	2	0.37
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	11	0.37
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.37
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.37
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.37
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.37
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.37
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.37
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	4	0.37
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	4	0.37
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	10	0.37
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	1	0.37
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	1	0.37
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	1	0.37
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	12	0.37
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	12	0.37
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	12	0.37
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	2	0.37
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	11	0.37
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.37
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.37
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.37
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.37
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.37
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.37
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	4	0.37
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	4	0.37
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	6	0.37
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	10	0.37
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	1	0.37
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	1	0.37
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	1	0.37
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	12	0.37
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	12	0.37
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	12	0.37
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	2	0.37
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	11	0.37
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.37
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.37
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.37
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.37
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.37
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.37
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	3	0.37
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	3	0.37
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	3	0.37
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	3	0.37
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	3	0.37
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	3	0.37
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	3	0.37
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	3	0.37
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	3	0.37
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	3	0.37
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	3	0.37
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	3	0.37
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	3	0.37
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	3	0.37
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	3	0.37
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	3	0.37
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	3	0.37
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	2	0.37
(1,73)	1:755:C:LEU:O	1:759:C:ASP:H	5	0.37
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	14	0.37
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	2	0.37
(1,47)	1:755:C:LEU:O	1:759:C:ASP:H	5	0.37
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	14	0.37
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	2	0.37
(1,21)	1:755:C:LEU:O	1:759:C:ASP:H	5	0.37
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	14	0.37
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	7	0.36
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	7	0.36
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	7	0.36
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	7	0.36
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	7	0.36
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	7	0.36
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	13	0.36
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	14	0.36
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	5	0.36
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	5	0.36
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	5	0.36
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	8	0.36
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	8	0.36
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	8	0.36
(2,1129)	1:705:A:VAL:HG11	1:706:A:ASN:HA	15	0.36
(2,1129)	1:705:A:VAL:HG12	1:706:A:ASN:HA	15	0.36
(2,1129)	1:705:A:VAL:HG13	1:706:A:ASN:HA	15	0.36
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	9	0.36
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.36
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.36
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.36
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.36
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.36
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.36
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	7	0.36
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	7	0.36
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	7	0.36
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	7	0.36
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	7	0.36
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	7	0.36
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	13	0.36
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	14	0.36
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	5	0.36
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	5	0.36
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	5	0.36
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	8	0.36
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	8	0.36
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	8	0.36
(2,723)	1:705:A:VAL:HG11	1:706:A:ASN:HA	15	0.36
(2,723)	1:705:A:VAL:HG12	1:706:A:ASN:HA	15	0.36
(2,723)	1:705:A:VAL:HG13	1:706:A:ASN:HA	15	0.36
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	9	0.36
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.36
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.36
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.36
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.36
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.36
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.36
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.36
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	7	0.36
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	7	0.36
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	7	0.36
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	7	0.36
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	7	0.36
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	7	0.36
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	13	0.36
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	14	0.36
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	5	0.36
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	5	0.36
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	5	0.36
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	8	0.36
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	8	0.36
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:705:A:VAL:HG11	1:706:A:ASN:HA	15	0.36
(2,317)	1:705:A:VAL:HG12	1:706:A:ASN:HA	15	0.36
(2,317)	1:705:A:VAL:HG13	1:706:A:ASN:HA	15	0.36
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	9	0.36
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.36
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.36
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.36
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.36
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.36
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.36
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.36
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	0.36
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	0.36
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	0.36
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	0.36
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	0.36
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	0.36
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	0.36
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	0.36
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	0.36
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	1	0.35
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	7	0.35
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	13	0.35
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.35
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.35
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.35
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	1	0.35
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	7	0.35
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	13	0.35
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.35
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.35
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.35
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	1	0.35
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	7	0.35
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	13	0.35
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.35
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.35
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.35
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	6	0.34
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	6	0.34
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	9	0.34
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	12	0.34
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	14	0.34
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	8	0.34
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	2	0.34
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.34
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	12	0.34
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	12	0.34
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	12	0.34
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.34
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	7	0.34
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	7	0.34
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.34
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.34
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	6	0.34
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	6	0.34
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	9	0.34
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	12	0.34
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	14	0.34
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	8	0.34
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	2	0.34
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.34
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	12	0.34
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	12	0.34
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	12	0.34
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	7	0.34
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	7	0.34
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.34
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.34
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	6	0.34
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	6	0.34
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	9	0.34
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	12	0.34
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	14	0.34
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	8	0.34
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	2	0.34
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	15	0.34
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	12	0.34
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	12	0.34
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	12	0.34
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.34
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	7	0.34
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	7	0.34
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.34
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.34
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	6	0.34
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	6	0.34
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	6	0.34
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	6	0.34
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	6	0.34
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	6	0.34
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	6	0.34
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	6	0.34
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	6	0.34
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	6	0.34
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	6	0.34
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	6	0.34
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	6	0.34
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	6	0.34
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	6	0.34
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	6	0.34
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	6	0.34
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	6	0.34
(1,59)	1:743:C:ASP:O	1:747:C:ARG:H	2	0.34
(1,33)	1:743:C:ASP:O	1:747:C:ARG:H	2	0.34
(1,7)	1:743:C:ASP:O	1:747:C:ARG:H	2	0.34
(2,1323)	1:784:A:LEU:H	1:781:A:ILE:HA	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	11	0.33
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	3	0.33
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	3	0.33
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	3	0.33
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	12	0.33
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	14	0.33
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	11	0.33
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	11	0.33
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	11	0.33
(2,1121)	1:704:A:LEU:HD11	1:707:A:ARG:HE	8	0.33
(2,1121)	1:704:A:LEU:HD12	1:707:A:ARG:HE	8	0.33
(2,1121)	1:704:A:LEU:HD13	1:707:A:ARG:HE	8	0.33
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.33
(2,917)	1:784:A:LEU:H	1:781:A:ILE:HA	7	0.33
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	11	0.33
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	3	0.33
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	3	0.33
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	3	0.33
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	12	0.33
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	14	0.33
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	11	0.33
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	11	0.33
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	11	0.33
(2,715)	1:704:A:LEU:HD11	1:707:A:ARG:HE	8	0.33
(2,715)	1:704:A:LEU:HD12	1:707:A:ARG:HE	8	0.33
(2,715)	1:704:A:LEU:HD13	1:707:A:ARG:HE	8	0.33
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.33
(2,511)	1:784:A:LEU:H	1:781:A:ILE:HA	7	0.33
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	11	0.33
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	15	0.33
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	3	0.33
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	3	0.33
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	3	0.33
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	12	0.33
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	14	0.33
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	11	0.33
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	11	0.33
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	11	0.33
(2,309)	1:704:A:LEU:HD11	1:707:A:ARG:HE	8	0.33
(2,309)	1:704:A:LEU:HD12	1:707:A:ARG:HE	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:704:A:LEU:HD13	1:707:A:ARG:HE	8	0.33
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.33
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.33
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.33
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.33
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.33
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.33
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.33
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	6	0.33
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	6	0.33
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	6	0.33
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	7	0.32
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	13	0.32
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	5	0.32
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	5	0.32
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	5	0.32
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	5	0.32
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	5	0.32
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	5	0.32
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	1	0.32
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.32
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	4	0.32
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.32
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.32
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.32
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.32
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.32
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.32
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.32
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.32
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.32
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.32
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.32
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.32
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.32
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.32
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.32
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.32
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.32
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.32
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.32
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.32
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.32
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	7	0.32
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	13	0.32
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	5	0.32
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	5	0.32
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	5	0.32
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	5	0.32
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	5	0.32
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	5	0.32
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	1	0.32
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.32
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	4	0.32
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.32
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.32
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.32
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.32
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.32
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.32
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.32
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.32
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.32
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.32
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.32
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.32
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.32
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.32
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.32
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.32
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.32
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.32
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.32
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.32
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.32
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.32
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	7	0.32
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	13	0.32
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	5	0.32
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	5	0.32
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	5	0.32
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	5	0.32
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	5	0.32
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	1	0.32
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	13	0.32
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	4	0.32
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.32
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.32
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.32
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.32
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.32
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.32
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.32
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.32
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.32
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.32
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.32
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.32
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.32
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.32
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.32
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.32
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.32
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.32
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.32
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.32
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.32
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.32
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	5	0.32
(2,72)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	5	0.32
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	5	0.32
(2,72)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	5	0.32
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	5	0.32
(2,72)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	5	0.32
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	5	0.32
(2,71)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	5	0.32
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	5	0.32
(2,71)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	5	0.32
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	5	0.32
(2,71)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	5	0.32
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB2	5	0.32
(2,70)	1:708:A:VAL:HG21	1:712:A:TYR:HB3	5	0.32
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB2	5	0.32
(2,70)	1:708:A:VAL:HG22	1:712:A:TYR:HB3	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB2	5	0.32
(2,70)	1:708:A:VAL:HG23	1:712:A:TYR:HB3	5	0.32
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.31
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	5	0.31
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	8	0.31
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	10	0.31
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	9	0.31
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	9	0.31
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	9	0.31
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	9	0.31
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	10	0.31
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	4	0.31
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	4	0.31
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	4	0.31
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	4	0.31
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	4	0.31
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	4	0.31
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.31
(2,1082)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.31
(2,1082)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.31
(2,1082)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.31
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.31
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	5	0.31
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	8	0.31
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	10	0.31
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	9	0.31
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	9	0.31
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	9	0.31
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	9	0.31
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	10	0.31
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	4	0.31
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	4	0.31
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	4	0.31
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	4	0.31
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	4	0.31
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	4	0.31
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.31
(2,676)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.31
(2,676)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.31
(2,676)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.31
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	12	0.31
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	8	0.31
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	10	0.31
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	9	0.31
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	9	0.31
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	9	0.31
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	9	0.31
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	10	0.31
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	4	0.31
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	4	0.31
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	4	0.31
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	4	0.31
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	4	0.31
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	4	0.31
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.31
(2,270)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.31
(2,270)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.31
(2,270)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.31
(1,62)	1:744:C:ARG:O	1:748:C:LEU:N	12	0.31
(1,36)	1:744:C:ARG:O	1:748:C:LEU:N	12	0.31
(1,10)	1:744:C:ARG:O	1:748:C:LEU:N	12	0.31
(2,1330)	1:784:A:LEU:HD21	1:781:A:ILE:HA	7	0.3
(2,1330)	1:784:A:LEU:HD22	1:781:A:ILE:HA	7	0.3
(2,1330)	1:784:A:LEU:HD23	1:781:A:ILE:HA	7	0.3
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	5	0.3
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.3
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	8	0.3
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	13	0.3
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	3	0.3
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	3	0.3
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	3	0.3
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	3	0.3
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	6	0.3
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	6	0.3
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	6	0.3
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	2	0.3
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	2	0.3
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	2	0.3
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	11	0.3
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	5	0.3
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	6	0.3
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	12	0.3
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	12	0.3
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	12	0.3
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	12	0.3
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	12	0.3
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	9	0.3
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	9	0.3
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	9	0.3
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.3
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.3
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	11	0.3
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	11	0.3
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.3
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.3
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.3
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.3
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.3
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.3
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.3
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.3
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.3
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.3
(2,924)	1:784:A:LEU:HD21	1:781:A:ILE:HA	7	0.3
(2,924)	1:784:A:LEU:HD22	1:781:A:ILE:HA	7	0.3
(2,924)	1:784:A:LEU:HD23	1:781:A:ILE:HA	7	0.3
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	5	0.3
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.3
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	8	0.3
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	13	0.3
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	3	0.3
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	3	0.3
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	3	0.3
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	3	0.3
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	6	0.3
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	6	0.3
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	6	0.3
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	2	0.3
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	2	0.3
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	11	0.3
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	5	0.3
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	6	0.3
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	12	0.3
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	12	0.3
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	12	0.3
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	12	0.3
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	12	0.3
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	12	0.3
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	9	0.3
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	9	0.3
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	9	0.3
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.3
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.3
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	11	0.3
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	11	0.3
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.3
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.3
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.3
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.3
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.3
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.3
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.3
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.3
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.3
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.3
(2,518)	1:784:A:LEU:HD21	1:781:A:ILE:HA	7	0.3
(2,518)	1:784:A:LEU:HD22	1:781:A:ILE:HA	7	0.3
(2,518)	1:784:A:LEU:HD23	1:781:A:ILE:HA	7	0.3
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	5	0.3
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	15	0.3
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	8	0.3
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	13	0.3
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	3	0.3
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	3	0.3
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	3	0.3
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	6	0.3
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	6	0.3
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	6	0.3
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	2	0.3
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	2	0.3
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	2	0.3
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	11	0.3
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	5	0.3
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	6	0.3
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	12	0.3
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	12	0.3
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	12	0.3
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	12	0.3
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	12	0.3
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	12	0.3
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	9	0.3
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	9	0.3
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	9	0.3
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.3
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.3
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	11	0.3
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	11	0.3
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.3
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.3
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.3
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.3
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.3
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.3
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.3
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.3
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.3
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.3
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	4	0.3
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	4	0.3
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	4	0.3
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	4	0.3
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	4	0.3
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	8	0.3
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	8	0.3
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	8	0.3
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	8	0.3
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	8	0.3
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	8	0.3
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	4	0.3
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	4	0.3
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	4	0.3
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	4	0.3
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	4	0.3
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	4	0.3
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	8	0.3
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	8	0.3
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	8	0.3
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	8	0.3
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	8	0.3
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	8	0.3
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	4	0.3
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	4	0.3
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	4	0.3
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	4	0.3
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	4	0.3
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	4	0.3
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	8	0.3
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	8	0.3
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	8	0.3
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	8	0.3
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	8	0.3
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	8	0.3
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	7	0.3
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	7	0.3
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	7	0.3
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	7	0.3
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	7	0.3
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	7	0.3
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	15	0.29
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	7	0.29
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	1	0.29
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	3	0.29
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	3	0.29
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.29
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.29
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.29
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.29
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	2	0.29
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	2	0.29
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	2	0.29
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	2	0.29
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	2	0.29
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	2	0.29
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.29
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	15	0.29
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	7	0.29
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	1	0.29
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	3	0.29
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	3	0.29
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	3	0.29
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.29
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.29
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.29
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.29
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	2	0.29
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	2	0.29
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	2	0.29
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	2	0.29
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	2	0.29
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	2	0.29
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.29
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	15	0.29
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	7	0.29
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	1	0.29
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	3	0.29
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	3	0.29
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	3	0.29
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.29
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.29
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.29
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.29
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	2	0.29
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	2	0.29
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	2	0.29
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	2	0.29
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	2	0.29
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.29
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	10	0.29
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	10	0.29
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	10	0.29
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	10	0.29
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	10	0.29
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	10	0.29
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	10	0.29
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	10	0.29
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	10	0.29
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	10	0.29
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	10	0.29
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	10	0.29
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	10	0.29
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	10	0.29
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	10	0.29
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	10	0.29
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	10	0.29
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	10	0.29
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.29
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.29
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.29
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.29
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.29
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.29
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.29
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.29
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.29
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.29
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.29
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.29
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.29
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.29
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.29
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.29
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.29
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.29
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.29
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.29
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.29
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.29
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.29
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.29
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.29
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.29
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.29
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.29
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.29
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.29
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.29
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.29
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.29
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.29
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.29
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	2	0.28
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	13	0.28
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	5	0.28
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	9	0.28
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	7	0.28
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	6	0.28
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	8	0.28
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	8	0.28
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	6	0.28
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	6	0.28
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	6	0.28
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.28
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.28
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.28
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.28
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.28
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.28
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.28
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.28
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.28
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	8	0.28
(2,1061)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	13	0.28
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.28
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.28
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	8	0.28
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	8	0.28
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	8	0.28
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	8	0.28
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	8	0.28
(2,976)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	8	0.28
(2,976)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	8	0.28
(2,976)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	8	0.28
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	2	0.28
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	13	0.28
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	5	0.28
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	9	0.28
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	7	0.28
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	6	0.28
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	8	0.28
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	8	0.28
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	6	0.28
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	6	0.28
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	6	0.28
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.28
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.28
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.28
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.28
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.28
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.28
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.28
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.28
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.28
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	8	0.28
(2,655)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	13	0.28
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.28
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	8	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	8	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	8	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	8	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	8	0.28
(2,570)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	8	0.28
(2,570)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	8	0.28
(2,570)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	8	0.28
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	2	0.28
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	13	0.28
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	5	0.28
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	9	0.28
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	7	0.28
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	6	0.28
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	8	0.28
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	8	0.28
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	6	0.28
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	6	0.28
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	6	0.28
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.28
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.28
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.28
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.28
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.28
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.28
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.28
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.28
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.28
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	8	0.28
(2,249)	1:692:A:LEU:HD12	1:696:A:ARG:HH12	13	0.28
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.28
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	8	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	8	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	8	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	8	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	8	0.28
(2,164)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	8	0.28
(2,164)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	8	0.28
(2,164)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	8	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	5	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	5	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	5	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	5	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	5	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	5	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	11	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	11	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	11	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	11	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	11	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	11	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.28
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.28
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.28
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	5	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	5	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	5	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	5	0.28
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	5	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	11	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	11	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	11	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	11	0.28
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	11	0.28
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	11	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.28
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.28
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.28
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.28
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	5	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	5	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	5	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	5	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	5	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	5	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	11	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	11	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	11	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	11	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	11	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	11	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	15	0.28
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	15	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	15	0.28
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	15	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	15	0.28
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	15	0.28
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.28
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.28
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.28
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.28
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.28
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.28
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.28
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.28
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.28
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.28
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.28
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.28
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.28
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.28
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.28
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.28
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.28
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.28
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.28
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.28
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.28
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.28
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.28
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.28
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.28
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.28
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.28
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.28
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.28
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.28
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.28
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.28
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.28
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.28
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.28
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.28
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.28
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.28
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.28
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.28
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.28
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.28
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.28
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.28
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.28
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.28
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.28
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.28
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.28
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.28
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.27
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	13	0.27
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	14	0.27
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	15	0.27
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	3	0.27
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	8	0.27
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	2	0.27
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	14	0.27
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	13	0.27
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	13	0.27
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	4	0.27
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	4	0.27
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	4	0.27
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	8	0.27
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	8	0.27
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	8	0.27
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	4	0.27
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.27
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.27
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.27
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.27
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.27
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.27
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.27
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.27
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.27
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.27
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.27
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.27
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.27
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.27
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.27
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	11	0.27
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.27
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.27
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.27
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.27
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.27
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.27
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.27
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.27
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.27
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.27
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.27
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.27
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	11	0.27
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.27
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	13	0.27
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	14	0.27
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	15	0.27
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	3	0.27
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	8	0.27
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	2	0.27
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	14	0.27
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	13	0.27
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	13	0.27
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	4	0.27
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	4	0.27
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	4	0.27
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	8	0.27
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	8	0.27
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	8	0.27
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	4	0.27
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.27
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.27
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.27
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.27
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.27
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.27
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.27
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.27
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.27
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.27
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.27
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.27
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.27
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.27
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.27
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	11	0.27
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.27
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.27
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.27
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.27
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.27
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.27
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.27
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.27
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.27
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.27
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.27
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.27
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	11	0.27
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	12	0.27
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	13	0.27
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	14	0.27
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	15	0.27
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	3	0.27
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	8	0.27
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	2	0.27
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	14	0.27
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	13	0.27
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	13	0.27
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	4	0.27
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	4	0.27
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	4	0.27
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	8	0.27
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	8	0.27
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	8	0.27
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	4	0.27
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.27
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.27
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.27
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.27
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.27
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.27
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.27
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.27
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.27
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.27
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.27
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.27
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.27
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.27
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	11	0.27
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.27
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.27
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.27
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.27
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.27
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.27
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.27
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.27
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.27
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.27
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.27
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.27
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	2	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	2	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	2	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	2	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	2	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	2	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	3	0.27
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	3	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	3	0.27
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	3	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	3	0.27
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	3	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	2	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	2	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	2	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	2	0.27
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	2	0.27
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	2	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	3	0.27
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	3	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	3	0.27
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	3	0.27
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	3	0.27
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	3	0.27
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	2	0.27
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	2	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	2	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	2	0.27
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	2	0.27
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	3	0.27
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	3	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	3	0.27
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	3	0.27
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	3	0.27
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	3	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.27
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.27
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.27
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.27
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.27
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.27
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.27
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.27
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.27
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.27
(1,74)	1:755:C:LEU:O	1:759:C:ASP:N	5	0.27
(1,48)	1:755:C:LEU:O	1:759:C:ASP:N	5	0.27
(1,22)	1:755:C:LEU:O	1:759:C:ASP:N	5	0.27
(2,1344)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	2	0.26
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	2	0.26
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	2	0.26
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	2	0.26
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	2	0.26
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	6	0.26
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	6	0.26
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	6	0.26
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	6	0.26
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	6	0.26
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	8	0.26
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	15	0.26
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	3	0.26
(2,1159)	1:709:A:ARG:H	1:707:A:ARG:H	9	0.26
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.26
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.26
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.26
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.26
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.26
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.26
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.26
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	3	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.26
(2,956)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.26
(2,938)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	2	0.26
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	2	0.26
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	2	0.26
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	2	0.26
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	2	0.26
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	6	0.26
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	6	0.26
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	6	0.26
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	6	0.26
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	6	0.26
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	6	0.26
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	8	0.26
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	15	0.26
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	3	0.26
(2,753)	1:709:A:ARG:H	1:707:A:ARG:H	9	0.26
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.26
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.26
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.26
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.26
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.26
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.26
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	3	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.26
(2,550)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.26
(2,532)	1:744:A:ARG:HH21	1:741:A:ASP:OD1	2	0.26
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	2	0.26
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	2	0.26
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	2	0.26
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	2	0.26
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	6	0.26
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	6	0.26
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	6	0.26
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	6	0.26
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	6	0.26
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	6	0.26
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	8	0.26
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	15	0.26
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	3	0.26
(2,347)	1:709:A:ARG:H	1:707:A:ARG:H	9	0.26
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.26
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.26
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.26
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.26
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.26
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.26
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.26
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	3	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.26
(2,144)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.26
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	2	0.26
(1,54)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.26
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	2	0.26
(1,28)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.26
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	2	0.26
(1,2)	1:740:C:ARG:O	1:744:C:ARG:N	14	0.26
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	5	0.25
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	6	0.25
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	9	0.25
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	11	0.25
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	14	0.25
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	7	0.25
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	7	0.25
(2,1200)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	5	0.25
(2,1200)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	5	0.25
(2,1200)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	5	0.25
(2,1165)	1:709:A:ARG:HE	1:709:A:ARG:H	8	0.25
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25
(2,1128)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.25
(2,1128)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.25
(2,1128)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.25
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.25
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.25
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.25
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.25
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.25
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.25
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.25
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	5	0.25
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	9	0.25
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	11	0.25
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	14	0.25
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	7	0.25
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	7	0.25
(2,794)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	5	0.25
(2,794)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	5	0.25
(2,794)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	5	0.25
(2,759)	1:709:A:ARG:HE	1:709:A:ARG:H	8	0.25
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25
(2,722)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.25
(2,722)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.25
(2,722)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.25
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.25
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.25
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.25
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.25
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.25
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.25
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.25
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	5	0.25
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD1	6	0.25
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	9	0.25
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	11	0.25
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	14	0.25
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	7	0.25
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	7	0.25
(2,388)	1:746:A:ILE:HG21	1:750:A:ASN:HD22	5	0.25
(2,388)	1:746:A:ILE:HG22	1:750:A:ASN:HD22	5	0.25
(2,388)	1:746:A:ILE:HG23	1:750:A:ASN:HD22	5	0.25
(2,353)	1:709:A:ARG:HE	1:709:A:ARG:H	8	0.25
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	7	0.25
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	7	0.25
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	7	0.25
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	7	0.25
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	7	0.25
(2,316)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.25
(2,316)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.25
(2,316)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.25
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.25
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.25
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.25
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.25
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.25
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.25
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.25
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.25
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.25
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.25
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.25
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.25
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.25
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.25
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.25
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.25
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.25
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.25
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.25
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.25
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.25
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.25
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.25
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.25
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.25
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.25
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.25
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.25
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.25
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.25
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	4	0.24
(2,1346)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	11	0.24
(2,1345)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	4	0.24
(2,1344)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	15	0.24
(2,1316)	1:782:A:VAL:HG21	1:779:A:THR:HA	5	0.24
(2,1316)	1:782:A:VAL:HG22	1:779:A:THR:HA	5	0.24
(2,1316)	1:782:A:VAL:HG23	1:779:A:THR:HA	5	0.24
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	10	0.24
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	1	0.24
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	1	0.24
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	1	0.24
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.24
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	3	0.24
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	3	0.24
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	9	0.24
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	13	0.24
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	14	0.24
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.24
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.24
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	12	0.24
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	12	0.24
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	13	0.24
(2,1052)	1:688:A:ILE:HG21	1:692:A:LEU:HG	15	0.24
(2,1052)	1:688:A:ILE:HG22	1:692:A:LEU:HG	15	0.24
(2,1052)	1:688:A:ILE:HG23	1:692:A:LEU:HG	15	0.24
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.24
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.24
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.24
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.24
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.24
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	4	0.24
(2,940)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	11	0.24
(2,939)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	4	0.24
(2,938)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	15	0.24
(2,910)	1:782:A:VAL:HG21	1:779:A:THR:HA	5	0.24
(2,910)	1:782:A:VAL:HG22	1:779:A:THR:HA	5	0.24
(2,910)	1:782:A:VAL:HG23	1:779:A:THR:HA	5	0.24
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	10	0.24
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	1	0.24
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	1	0.24
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.24
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	3	0.24
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	3	0.24
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	9	0.24
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	13	0.24
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	14	0.24
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.24
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.24
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	12	0.24
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	12	0.24
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	13	0.24
(2,646)	1:688:A:ILE:HG21	1:692:A:LEU:HG	15	0.24
(2,646)	1:688:A:ILE:HG22	1:692:A:LEU:HG	15	0.24
(2,646)	1:688:A:ILE:HG23	1:692:A:LEU:HG	15	0.24
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.24
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.24
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.24
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.24
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.24
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE2	4	0.24
(2,534)	1:770:A:ARG:HH11	1:773:A:ASP:OD2	11	0.24
(2,533)	1:761:A:ARG:HH22	1:758:A:ASP:OD1	4	0.24
(2,532)	1:744:A:ARG:HH11	1:741:A:ASP:OD2	15	0.24
(2,504)	1:782:A:VAL:HG21	1:779:A:THR:HA	5	0.24
(2,504)	1:782:A:VAL:HG22	1:779:A:THR:HA	5	0.24
(2,504)	1:782:A:VAL:HG23	1:779:A:THR:HA	5	0.24
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	10	0.24
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	1	0.24
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	1	0.24
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	1	0.24
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	15	0.24
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	3	0.24
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	3	0.24
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	9	0.24
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	13	0.24
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	14	0.24
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.24
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.24
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	12	0.24
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	12	0.24
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,240)	1:688:A:ILE:HG21	1:692:A:LEU:HG	15	0.24
(2,240)	1:688:A:ILE:HG22	1:692:A:LEU:HG	15	0.24
(2,240)	1:688:A:ILE:HG23	1:692:A:LEU:HG	15	0.24
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.24
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.24
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.24
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.24
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.24
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	14	0.24
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	14	0.24
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	14	0.24
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	14	0.24
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	14	0.24
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	14	0.24
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	14	0.24
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	14	0.24
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	14	0.24
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	14	0.24
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	14	0.24
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	14	0.24
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	14	0.24
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	14	0.24
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	14	0.24
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	14	0.24
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	14	0.24
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	14	0.24
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.24
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.24
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.24
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.24
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.24
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.24
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.24
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.24
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.24
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.24
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.24
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.24
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.24
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.24
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.24
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.24
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.24
(2,1344)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	10	0.23
(2,1323)	1:784:A:LEU:H	1:781:A:ILE:HA	8	0.23
(2,1316)	1:782:A:VAL:HG21	1:779:A:THR:HA	15	0.23
(2,1316)	1:782:A:VAL:HG22	1:779:A:THR:HA	15	0.23
(2,1316)	1:782:A:VAL:HG23	1:779:A:THR:HA	15	0.23
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	9	0.23
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	4	0.23
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	4	0.23
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	4	0.23
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	12	0.23
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	12	0.23
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	12	0.23
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	12	0.23
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	12	0.23
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	12	0.23
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	3	0.23
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	3	0.23
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	3	0.23
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	3	0.23
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	3	0.23
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	3	0.23
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.23
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.23
(2,1100)	1:701:A:VAL:HG21	1:698:A:VAL:HA	7	0.23
(2,1100)	1:701:A:VAL:HG22	1:698:A:VAL:HA	7	0.23
(2,1100)	1:701:A:VAL:HG23	1:698:A:VAL:HA	7	0.23
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.23
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.23
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.23
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	6	0.23
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.23
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.23
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.23
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.23
(2,938)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	10	0.23
(2,917)	1:784:A:LEU:H	1:781:A:ILE:HA	8	0.23
(2,910)	1:782:A:VAL:HG21	1:779:A:THR:HA	15	0.23
(2,910)	1:782:A:VAL:HG22	1:779:A:THR:HA	15	0.23
(2,910)	1:782:A:VAL:HG23	1:779:A:THR:HA	15	0.23
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	4	0.23
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	4	0.23
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	4	0.23
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	12	0.23
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	12	0.23
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	12	0.23
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	12	0.23
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	12	0.23
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	12	0.23
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	3	0.23
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	3	0.23
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	3	0.23
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	3	0.23
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	3	0.23
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	3	0.23
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.23
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.23
(2,694)	1:701:A:VAL:HG21	1:698:A:VAL:HA	7	0.23
(2,694)	1:701:A:VAL:HG22	1:698:A:VAL:HA	7	0.23
(2,694)	1:701:A:VAL:HG23	1:698:A:VAL:HA	7	0.23
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.23
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.23
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.23
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	6	0.23
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.23
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.23
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.23
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.23
(2,532)	1:744:A:ARG:HH11	1:741:A:ASP:OD1	10	0.23
(2,511)	1:784:A:LEU:H	1:781:A:ILE:HA	8	0.23
(2,504)	1:782:A:VAL:HG21	1:779:A:THR:HA	15	0.23
(2,504)	1:782:A:VAL:HG22	1:779:A:THR:HA	15	0.23
(2,504)	1:782:A:VAL:HG23	1:779:A:THR:HA	15	0.23
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	9	0.23
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	4	0.23
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	4	0.23
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	4	0.23
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	12	0.23
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	12	0.23
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	12	0.23
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	12	0.23
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	12	0.23
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	3	0.23
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	3	0.23
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	3	0.23
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	3	0.23
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	3	0.23
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	3	0.23
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.23
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.23
(2,288)	1:701:A:VAL:HG21	1:698:A:VAL:HA	7	0.23
(2,288)	1:701:A:VAL:HG22	1:698:A:VAL:HA	7	0.23
(2,288)	1:701:A:VAL:HG23	1:698:A:VAL:HA	7	0.23
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.23
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.23
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.23
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	6	0.23
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.23
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.23
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.23
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.23
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	9	0.23
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	9	0.23
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	9	0.23
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	9	0.23
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	9	0.23
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	9	0.23
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	9	0.23
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	9	0.23
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	9	0.23
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	9	0.23
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	9	0.23
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	9	0.23
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	9	0.23
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	9	0.23
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	9	0.23
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	9	0.23
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	9	0.23
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	9	0.23
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	1	0.22
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	1	0.22
(2,1295)	1:779:A:THR:H	1:776:A:LEU:HA	3	0.22
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:774:A:LEU:H	1:764:A:SER:HA	9	0.22
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	3	0.22
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	15	0.22
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	1	0.22
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.22
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	2	0.22
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	2	0.22
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	2	0.22
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.22
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.22
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	9	0.22
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	9	0.22
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	9	0.22
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	9	0.22
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	9	0.22
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	9	0.22
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.22
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.22
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.22
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.22
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.22
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.22
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.22
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.22
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.22
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.22
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.22
(2,953)	1:664:A:ASP:H	1:663:A:LEU:H	8	0.22
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.22
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.22
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.22
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.22
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.22
(2,947)	1:663:A:LEU:H	1:664:A:ASP:H	8	0.22
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	1	0.22
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	1	0.22
(2,889)	1:779:A:THR:H	1:776:A:LEU:HA	3	0.22
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	3	0.22
(2,860)	1:774:A:LEU:H	1:764:A:SER:HA	9	0.22
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	3	0.22
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	1	0.22
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.22
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	2	0.22
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	2	0.22
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	2	0.22
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.22
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.22
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	9	0.22
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	9	0.22
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	9	0.22
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	9	0.22
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	9	0.22
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	9	0.22
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.22
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.22
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.22
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.22
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.22
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.22
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.22
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.22
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.22
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.22
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.22
(2,547)	1:664:A:ASP:H	1:663:A:LEU:H	8	0.22
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.22
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.22
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.22
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.22
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.22
(2,541)	1:663:A:LEU:H	1:664:A:ASP:H	8	0.22
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	1	0.22
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	1	0.22
(2,483)	1:779:A:THR:H	1:776:A:LEU:HA	3	0.22
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	3	0.22
(2,454)	1:774:A:LEU:H	1:764:A:SER:HA	9	0.22
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	3	0.22
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	15	0.22
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	1	0.22
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	15	0.22
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	2	0.22
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	2	0.22
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.22
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	15	0.22
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	9	0.22
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	9	0.22
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	9	0.22
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	9	0.22
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	9	0.22
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	9	0.22
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.22
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.22
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.22
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.22
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.22
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.22
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.22
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.22
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.22
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.22
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.22
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.22
(2,141)	1:664:A:ASP:H	1:663:A:LEU:H	8	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.22
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.22
(2,135)	1:663:A:LEU:H	1:664:A:ASP:H	8	0.22
(1,75)	1:756:C:ILE:O	1:760:C:LEU:H	4	0.22
(1,67)	1:747:C:ARG:O	1:751:C:GLY:H	5	0.22
(1,60)	1:743:C:ASP:O	1:747:C:ARG:N	12	0.22
(1,49)	1:756:C:ILE:O	1:760:C:LEU:H	4	0.22
(1,41)	1:747:C:ARG:O	1:751:C:GLY:H	5	0.22
(1,34)	1:743:C:ASP:O	1:747:C:ARG:N	12	0.22
(1,23)	1:756:C:ILE:O	1:760:C:LEU:H	4	0.22
(1,15)	1:747:C:ARG:O	1:751:C:GLY:H	5	0.22
(1,8)	1:743:C:ASP:O	1:747:C:ARG:N	12	0.22
(2,1337)	1:785:A:LEU:HD21	1:782:A:VAL:HA	8	0.21
(2,1337)	1:785:A:LEU:HD22	1:782:A:VAL:HA	8	0.21
(2,1337)	1:785:A:LEU:HD23	1:782:A:VAL:HA	8	0.21
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	14	0.21
(2,1311)	1:782:A:VAL:H	1:779:A:THR:HA	6	0.21
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	8	0.21
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	8	0.21
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	8	0.21
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	6	0.21
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	7	0.21
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	13	0.21
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	13	0.21
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	13	0.21
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	13	0.21
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	13	0.21
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	13	0.21
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	15	0.21
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	15	0.21
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	15	0.21
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	15	0.21
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	15	0.21
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	15	0.21
(2,1261)	1:773:A:ASP:H	1:770:A:ARG:HD2	6	0.21
(2,1261)	1:773:A:ASP:H	1:770:A:ARG:HD3	6	0.21
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	10	0.21
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	10	0.21
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	3	0.21
(2,1235)	1:755:A:LEU:HD21	1:759:A:ASP:HB2	3	0.21
(2,1235)	1:755:A:LEU:HD22	1:759:A:ASP:HB2	3	0.21
(2,1235)	1:755:A:LEU:HD23	1:759:A:ASP:HB2	3	0.21
(2,1234)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	10	0.21
(2,1234)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	10	0.21
(2,1234)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	10	0.21
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	10	0.21
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	10	0.21
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	5	0.21
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	10	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD11	6	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD12	6	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD13	6	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD21	6	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD22	6	0.21
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD23	6	0.21
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.21
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.21
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.21
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.21
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.21
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.21
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.21
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.21
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.21
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	11	0.21
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	3	0.21
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	3	0.21
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	3	0.21
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	3	0.21
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	3	0.21
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	3	0.21
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	3	0.21
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	3	0.21
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	3	0.21
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.21
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	15	0.21
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	15	0.21
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	15	0.21
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.21
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.21
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.21
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.21
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.21
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.21
(2,931)	1:785:A:LEU:HD21	1:782:A:VAL:HA	8	0.21
(2,931)	1:785:A:LEU:HD22	1:782:A:VAL:HA	8	0.21
(2,931)	1:785:A:LEU:HD23	1:782:A:VAL:HA	8	0.21
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	14	0.21
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	14	0.21
(2,905)	1:782:A:VAL:H	1:779:A:THR:HA	6	0.21
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	8	0.21
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	8	0.21
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	8	0.21
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	6	0.21
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	7	0.21
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	13	0.21
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	13	0.21
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	13	0.21
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	13	0.21
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	13	0.21
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	13	0.21
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	15	0.21
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	15	0.21
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	15	0.21
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	15	0.21
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	15	0.21
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	15	0.21
(2,855)	1:773:A:ASP:H	1:770:A:ARG:HD2	6	0.21
(2,855)	1:773:A:ASP:H	1:770:A:ARG:HD3	6	0.21
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	10	0.21
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	10	0.21
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	3	0.21
(2,829)	1:755:A:LEU:HD21	1:759:A:ASP:HB2	3	0.21
(2,829)	1:755:A:LEU:HD22	1:759:A:ASP:HB2	3	0.21
(2,829)	1:755:A:LEU:HD23	1:759:A:ASP:HB2	3	0.21
(2,828)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	10	0.21
(2,828)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	10	0.21
(2,828)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	10	0.21
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	10	0.21
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	10	0.21
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	10	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD11	6	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD12	6	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD13	6	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD21	6	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD22	6	0.21
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD23	6	0.21
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.21
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.21
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.21
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.21
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.21
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	11	0.21
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	3	0.21
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	3	0.21
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	3	0.21
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	3	0.21
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	3	0.21
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	3	0.21
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	3	0.21
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	3	0.21
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	3	0.21
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.21
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	15	0.21
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	15	0.21
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.21
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.21
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.21
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.21
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.21
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.21
(2,525)	1:785:A:LEU:HD21	1:782:A:VAL:HA	8	0.21
(2,525)	1:785:A:LEU:HD22	1:782:A:VAL:HA	8	0.21
(2,525)	1:785:A:LEU:HD23	1:782:A:VAL:HA	8	0.21
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	14	0.21
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	14	0.21
(2,499)	1:782:A:VAL:H	1:779:A:THR:HA	6	0.21
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	8	0.21
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	8	0.21
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	8	0.21
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	6	0.21
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	7	0.21
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	13	0.21
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	13	0.21
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	13	0.21
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	13	0.21
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	13	0.21
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	13	0.21
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	15	0.21
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	15	0.21
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	15	0.21
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	15	0.21
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	15	0.21
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	15	0.21
(2,449)	1:773:A:ASP:H	1:770:A:ARG:HD2	6	0.21
(2,449)	1:773:A:ASP:H	1:770:A:ARG:HD3	6	0.21
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	10	0.21
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	10	0.21
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:755:A:LEU:HD21	1:759:A:ASP:HB2	3	0.21
(2,423)	1:755:A:LEU:HD22	1:759:A:ASP:HB2	3	0.21
(2,423)	1:755:A:LEU:HD23	1:759:A:ASP:HB2	3	0.21
(2,422)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	10	0.21
(2,422)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	10	0.21
(2,422)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	10	0.21
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	10	0.21
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	10	0.21
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	5	0.21
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	10	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD11	6	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD12	6	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD13	6	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD21	6	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD22	6	0.21
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD23	6	0.21
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.21
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.21
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.21
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.21
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.21
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	11	0.21
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	3	0.21
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	3	0.21
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	3	0.21
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	3	0.21
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	3	0.21
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	3	0.21
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	3	0.21
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	3	0.21
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.21
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	15	0.21
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	15	0.21
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	15	0.21
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.21
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.21
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.21
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.21
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.21
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.21
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	7	0.21
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	7	0.21
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	7	0.21
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	7	0.21
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	7	0.21
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	7	0.21
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	13	0.21
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	13	0.21
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	13	0.21
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	13	0.21
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	13	0.21
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	13	0.21
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	7	0.21
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	7	0.21
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	7	0.21
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	7	0.21
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	7	0.21
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	7	0.21
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	13	0.21
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	13	0.21
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	13	0.21
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	13	0.21
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	13	0.21
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	7	0.21
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	7	0.21
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	7	0.21
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	7	0.21
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	7	0.21
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	7	0.21
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	13	0.21
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	13	0.21
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	13	0.21
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	13	0.21
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	13	0.21
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	13	0.21
(1,67)	1:747:C:ARG:O	1:751:C:GLY:H	9	0.21
(1,41)	1:747:C:ARG:O	1:751:C:GLY:H	9	0.21
(1,15)	1:747:C:ARG:O	1:751:C:GLY:H	9	0.21
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	13	0.2
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	1	0.2
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	1	0.2
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	1	0.2
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	1	0.2
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	1	0.2
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	1	0.2
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	9	0.2
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	9	0.2
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB2	8	0.2
(2,1220)	1:754:A:ALA:H	1:750:A:ASN:HB3	8	0.2
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	8	0.2
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	14	0.2
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	13	0.2
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	11	0.2
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	11	0.2
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	11	0.2
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	9	0.2
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	9	0.2
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	9	0.2
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	9	0.2
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	9	0.2
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	1	0.2
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	1	0.2
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	1	0.2
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	7	0.2
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	7	0.2
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	7	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD11	8	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD12	8	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD13	8	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD21	8	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD22	8	0.2
(2,1149)	1:707:A:ARG:HE	1:704:A:LEU:HD23	8	0.2
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.2
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.2
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.2
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.2
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.2
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.2
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.2
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.2
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.2
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.2
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.2
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.2
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.2
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.2
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	13	0.2
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	1	0.2
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	1	0.2
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	1	0.2
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	1	0.2
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	1	0.2
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	1	0.2
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	9	0.2
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	9	0.2
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB2	8	0.2
(2,814)	1:754:A:ALA:H	1:750:A:ASN:HB3	8	0.2
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	14	0.2
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	13	0.2
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	11	0.2
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	11	0.2
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	11	0.2
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	9	0.2
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	9	0.2
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	9	0.2
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	9	0.2
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	9	0.2
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	9	0.2
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	1	0.2
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	1	0.2
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	1	0.2
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	7	0.2
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	7	0.2
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	7	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD11	8	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD12	8	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD13	8	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD21	8	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD22	8	0.2
(2,743)	1:707:A:ARG:HE	1:704:A:LEU:HD23	8	0.2
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.2
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.2
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.2
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.2
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.2
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.2
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.2
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.2
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.2
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.2
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.2
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.2
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.2
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.2
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	13	0.2
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	1	0.2
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	1	0.2
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	1	0.2
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	1	0.2
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	1	0.2
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	9	0.2
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	9	0.2
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB2	8	0.2
(2,408)	1:754:A:ALA:H	1:750:A:ASN:HB3	8	0.2
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	8	0.2
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	14	0.2
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	13	0.2
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	11	0.2
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	11	0.2
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	11	0.2
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	9	0.2
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	9	0.2
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	9	0.2
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	9	0.2
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	9	0.2
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	9	0.2
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	1	0.2
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	1	0.2
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	1	0.2
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	7	0.2
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	7	0.2
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	7	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD11	8	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD12	8	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD13	8	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD21	8	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD22	8	0.2
(2,337)	1:707:A:ARG:HE	1:704:A:LEU:HD23	8	0.2
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.2
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.2
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.2
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.2
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.2
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.2
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.2
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.2
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.2
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.2
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.2
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.2
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.2
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.2
(1,69)	1:753:C:LEU:O	1:757:C:TRP:H	1	0.2
(1,43)	1:753:C:LEU:O	1:757:C:TRP:H	1	0.2
(1,17)	1:753:C:LEU:O	1:757:C:TRP:H	1	0.2
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	10	0.19
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	10	0.19
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	10	0.19
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	10	0.19
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	10	0.19
(2,1289)	1:778:A:VAL:H	1:775:A:LEU:HA	12	0.19
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	1	0.19
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	1	0.19
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	1	0.19
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	1	0.19
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	1	0.19
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	1	0.19
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	2	0.19
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	2	0.19
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	2	0.19
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	2	0.19
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	2	0.19
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	2	0.19
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	4	0.19
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	3	0.19
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	12	0.19
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB2	14	0.19
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB3	14	0.19
(2,1190)	1:746:A:ILE:H	1:742:A:ARG:HA	10	0.19
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	10	0.19
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	10	0.19
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	10	0.19
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	14	0.19
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	14	0.19
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.19
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.19
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.19
(2,1150)	1:708:A:VAL:H	1:705:A:VAL:HA	7	0.19
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.19
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.19
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.19
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.19
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.19
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.19
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.19
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.19
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.19
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.19
(2,1078)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.19
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	14	0.19
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	14	0.19
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	14	0.19
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	14	0.19
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	14	0.19
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	14	0.19
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.19
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.19
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.19
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.19
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.19
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.19
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	15	0.19
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	15	0.19
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	15	0.19
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	15	0.19
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	15	0.19
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	15	0.19
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.19
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.19
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.19
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.19
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.19
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.19
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.19
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.19
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.19
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.19
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.19
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.19
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.19
(2,973)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.19
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.19
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.19
(2,957)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	10	0.19
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	10	0.19
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	10	0.19
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	10	0.19
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	10	0.19
(2,883)	1:778:A:VAL:H	1:775:A:LEU:HA	12	0.19
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	1	0.19
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	1	0.19
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	1	0.19
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	1	0.19
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	1	0.19
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	1	0.19
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	2	0.19
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	2	0.19
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	2	0.19
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	2	0.19
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	2	0.19
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	2	0.19
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	4	0.19
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	3	0.19
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	12	0.19
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB2	14	0.19
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB3	14	0.19
(2,784)	1:746:A:ILE:H	1:742:A:ARG:HA	10	0.19
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	10	0.19
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	10	0.19
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	10	0.19
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	14	0.19
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	14	0.19
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	14	0.19
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.19
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.19
(2,744)	1:708:A:VAL:H	1:705:A:VAL:HA	7	0.19
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.19
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.19
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.19
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.19
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.19
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.19
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.19
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.19
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.19
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.19
(2,672)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.19
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	14	0.19
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	14	0.19
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	14	0.19
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	14	0.19
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	14	0.19
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	14	0.19
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.19
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.19
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.19
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.19
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.19
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.19
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	15	0.19
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	15	0.19
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	15	0.19
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	15	0.19
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	15	0.19
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	15	0.19
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.19
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.19
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.19
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.19
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.19
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.19
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.19
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.19
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.19
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.19
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.19
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.19
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.19
(2,567)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.19
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.19
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.19
(2,551)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	10	0.19
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	10	0.19
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	10	0.19
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	10	0.19
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	10	0.19
(2,477)	1:778:A:VAL:H	1:775:A:LEU:HA	12	0.19
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	1	0.19
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	1	0.19
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	1	0.19
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	1	0.19
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	1	0.19
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	1	0.19
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	2	0.19
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	2	0.19
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	2	0.19
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	2	0.19
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	2	0.19
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	2	0.19
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	4	0.19
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	11	0.19
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	3	0.19
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	12	0.19
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB2	14	0.19
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB3	14	0.19
(2,378)	1:746:A:ILE:H	1:742:A:ARG:HA	10	0.19
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	10	0.19
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	10	0.19
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	10	0.19
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	14	0.19
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	14	0.19
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	14	0.19
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	15	0.19
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	15	0.19
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	15	0.19
(2,338)	1:708:A:VAL:H	1:705:A:VAL:HA	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.19
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.19
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.19
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.19
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.19
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.19
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.19
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.19
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.19
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.19
(2,266)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.19
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	14	0.19
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	14	0.19
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	14	0.19
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	14	0.19
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	14	0.19
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	14	0.19
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.19
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.19
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.19
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.19
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.19
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.19
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	15	0.19
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	15	0.19
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	15	0.19
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	15	0.19
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	15	0.19
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	15	0.19
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.19
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.19
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.19
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.19
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.19
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.19
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.19
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.19
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.19
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.19
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.19
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.19
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.19
(2,161)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.19
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.19
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.19
(2,145)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.19
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.19
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.19
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.19
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.19
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.19
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.19
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.19
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.19
(1,69)	1:753:C:LEU:O	1:757:C:TRP:H	11	0.19
(1,55)	1:741:C:ASP:O	1:745:C:SER:H	13	0.19
(1,43)	1:753:C:LEU:O	1:757:C:TRP:H	11	0.19
(1,29)	1:741:C:ASP:O	1:745:C:SER:H	13	0.19
(1,17)	1:753:C:LEU:O	1:757:C:TRP:H	11	0.19
(1,3)	1:741:C:ASP:O	1:745:C:SER:H	13	0.19
(2,1341)	1:787:A:ARG:H	1:786:A:GLY:H	5	0.18
(2,1340)	1:786:A:GLY:H	1:787:A:ARG:H	5	0.18
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	6	0.18
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	9	0.18
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	5	0.18
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	5	0.18
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	5	0.18
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	5	0.18
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	5	0.18
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	5	0.18
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.18
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.18
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.18
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.18
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.18
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.18
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	3	0.18
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	3	0.18
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	15	0.18
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	15	0.18
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	4	0.18
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	14	0.18
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	15	0.18
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	15	0.18
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	4	0.18
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	9	0.18
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	14	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	4	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	4	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	4	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	4	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	4	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	4	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	9	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	9	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	9	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	9	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	9	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	9	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	10	0.18
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	10	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	10	0.18
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	10	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	10	0.18
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	10	0.18
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB2	12	0.18
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB3	12	0.18
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	15	0.18
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	15	0.18
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.18
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.18
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.18
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.18
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.18
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.18
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	14	0.18
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	14	0.18
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	14	0.18
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	14	0.18
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	14	0.18
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	14	0.18
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	14	0.18
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	14	0.18
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	8	0.18
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	8	0.18
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	8	0.18
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	8	0.18
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	8	0.18
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	8	0.18
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	5	0.18
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.18
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(2,1022)	1:682:A:ILE:HG21	1:685:A:PHE:HB2	15	0.18
(2,1022)	1:682:A:ILE:HG21	1:685:A:PHE:HB3	15	0.18
(2,1022)	1:682:A:ILE:HG22	1:685:A:PHE:HB2	15	0.18
(2,1022)	1:682:A:ILE:HG22	1:685:A:PHE:HB3	15	0.18
(2,1022)	1:682:A:ILE:HG23	1:685:A:PHE:HB2	15	0.18
(2,1022)	1:682:A:ILE:HG23	1:685:A:PHE:HB3	15	0.18
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.18
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.18
(2,962)	1:666:A:TRP:H	1:663:A:LEU:HA	8	0.18
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.18
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.18
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.18
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.18
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.18
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.18
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.18
(2,935)	1:787:A:ARG:H	1:786:A:GLY:H	5	0.18
(2,934)	1:786:A:GLY:H	1:787:A:ARG:H	5	0.18
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	9	0.18
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	5	0.18
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	5	0.18
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	5	0.18
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	5	0.18
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	5	0.18
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	5	0.18
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.18
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.18
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.18
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.18
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.18
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.18
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	3	0.18
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	3	0.18
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	15	0.18
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	15	0.18
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	4	0.18
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.18
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	14	0.18
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	15	0.18
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	15	0.18
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	4	0.18
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	9	0.18
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	14	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	4	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	4	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	4	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	4	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	4	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	4	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	9	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	9	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	9	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	9	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	9	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	9	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	10	0.18
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	10	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	10	0.18
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	10	0.18
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	10	0.18
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB2	12	0.18
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB3	12	0.18
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	15	0.18
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	15	0.18
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.18
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.18
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.18
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.18
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.18
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.18
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	14	0.18
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	14	0.18
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	14	0.18
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	14	0.18
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	14	0.18
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	14	0.18
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	14	0.18
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	14	0.18
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	14	0.18
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	8	0.18
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	8	0.18
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	8	0.18
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	8	0.18
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	8	0.18
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	8	0.18
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	5	0.18
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.18
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(2,616)	1:682:A:ILE:HG21	1:685:A:PHE:HB2	15	0.18
(2,616)	1:682:A:ILE:HG21	1:685:A:PHE:HB3	15	0.18
(2,616)	1:682:A:ILE:HG22	1:685:A:PHE:HB2	15	0.18
(2,616)	1:682:A:ILE:HG22	1:685:A:PHE:HB3	15	0.18
(2,616)	1:682:A:ILE:HG23	1:685:A:PHE:HB2	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:682:A:ILE:HG23	1:685:A:PHE:HB3	15	0.18
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.18
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.18
(2,556)	1:666:A:TRP:H	1:663:A:LEU:HA	8	0.18
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.18
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.18
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.18
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.18
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.18
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.18
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.18
(2,529)	1:787:A:ARG:H	1:786:A:GLY:H	5	0.18
(2,528)	1:786:A:GLY:H	1:787:A:ARG:H	5	0.18
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	6	0.18
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	9	0.18
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	5	0.18
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	5	0.18
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	5	0.18
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	5	0.18
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	5	0.18
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	5	0.18
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	11	0.18
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	11	0.18
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	11	0.18
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	11	0.18
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	11	0.18
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	11	0.18
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	3	0.18
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	3	0.18
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	15	0.18
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	15	0.18
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	4	0.18
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	10	0.18
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	14	0.18
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	15	0.18
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	15	0.18
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	9	0.18
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	14	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	4	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	4	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	4	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	4	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	4	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	4	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	9	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	9	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	9	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	9	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	9	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	9	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	10	0.18
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	10	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	10	0.18
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	10	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	10	0.18
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	10	0.18
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB2	12	0.18
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB3	12	0.18
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	15	0.18
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	15	0.18
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.18
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.18
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.18
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.18
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.18
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.18
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	14	0.18
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	14	0.18
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	14	0.18
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	14	0.18
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	14	0.18
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	14	0.18
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	14	0.18
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	14	0.18
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	14	0.18
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	8	0.18
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	8	0.18
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	8	0.18
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	8	0.18
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	8	0.18
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	5	0.18
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.18
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(2,210)	1:682:A:ILE:HG21	1:685:A:PHE:HB2	15	0.18
(2,210)	1:682:A:ILE:HG21	1:685:A:PHE:HB3	15	0.18
(2,210)	1:682:A:ILE:HG22	1:685:A:PHE:HB2	15	0.18
(2,210)	1:682:A:ILE:HG22	1:685:A:PHE:HB3	15	0.18
(2,210)	1:682:A:ILE:HG23	1:685:A:PHE:HB2	15	0.18
(2,210)	1:682:A:ILE:HG23	1:685:A:PHE:HB3	15	0.18
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.18
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.18
(2,150)	1:666:A:TRP:H	1:663:A:LEU:HA	8	0.18
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.18
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.18
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.18
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.18
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.18
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.18
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.18
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	1	0.18
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	1	0.18
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	1	0.18
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	1	0.18
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	1	0.18
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	1	0.18
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	1	0.18
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	1	0.18
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	1	0.18
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	1	0.18
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	1	0.18
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	1	0.18
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	1	0.18
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	1	0.18
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	1	0.18
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	1	0.18
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	1	0.18
(1,76)	1:756:C:ILE:O	1:760:C:LEU:N	4	0.18
(1,50)	1:756:C:ILE:O	1:760:C:LEU:N	4	0.18
(1,24)	1:756:C:ILE:O	1:760:C:LEU:N	4	0.18
(2,1344)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	7	0.17
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	8	0.17
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	8	0.17
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	8	0.17
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	8	0.17
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	8	0.17
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	8	0.17
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	11	0.17
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	11	0.17
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	11	0.17
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	4	0.17
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	4	0.17
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	4	0.17
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	4	0.17
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	4	0.17
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	4	0.17
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	14	0.17
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	14	0.17
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	14	0.17
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	14	0.17
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	14	0.17
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	14	0.17
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.17
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.17
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	9	0.17
(2,1234)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	9	0.17
(2,1234)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	9	0.17
(2,1234)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	9	0.17
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	9	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	9	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	9	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	9	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	9	0.17
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	10	0.17
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	10	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	10	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	10	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	10	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	10	0.17
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	15	0.17
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	15	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	15	0.17
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	15	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	15	0.17
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	15	0.17
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	6	0.17
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	6	0.17
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.17
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.17
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.17
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.17
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.17
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.17
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	13	0.17
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	13	0.17
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	13	0.17
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	13	0.17
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	13	0.17
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	13	0.17
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.17
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.17
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.17
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.17
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.17
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.17
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.17
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.17
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.17
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.17
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	3	0.17
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	3	0.17
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	3	0.17
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	15	0.17
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	15	0.17
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	15	0.17
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.17
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.17
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.17
(2,952)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.17
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.17
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.17
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.17
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.17
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.17
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.17
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.17
(2,938)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	7	0.17
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	8	0.17
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	8	0.17
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	8	0.17
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	8	0.17
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	8	0.17
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	8	0.17
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	11	0.17
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	11	0.17
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	11	0.17
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	4	0.17
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	4	0.17
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	4	0.17
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	4	0.17
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	4	0.17
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	14	0.17
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	14	0.17
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	14	0.17
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	14	0.17
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	14	0.17
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	14	0.17
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.17
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.17
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	9	0.17
(2,828)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	9	0.17
(2,828)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	9	0.17
(2,828)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	9	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	9	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	9	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	9	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	9	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	9	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	9	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	10	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	10	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	10	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	10	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	10	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	10	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	15	0.17
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	15	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	15	0.17
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	15	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	15	0.17
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	15	0.17
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	6	0.17
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	6	0.17
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.17
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.17
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.17
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.17
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.17
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.17
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	13	0.17
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	13	0.17
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	13	0.17
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	13	0.17
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	13	0.17
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.17
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.17
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.17
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.17
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.17
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.17
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.17
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.17
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.17
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.17
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.17
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	3	0.17
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	3	0.17
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	3	0.17
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	15	0.17
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	15	0.17
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	15	0.17
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.17
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.17
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.17
(2,546)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.17
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.17
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.17
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.17
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.17
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.17
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.17
(2,532)	1:744:A:ARG:HH22	1:741:A:ASP:OD2	7	0.17
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	8	0.17
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	8	0.17
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	8	0.17
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	8	0.17
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	8	0.17
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	8	0.17
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	11	0.17
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	11	0.17
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	11	0.17
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	4	0.17
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	4	0.17
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	4	0.17
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	4	0.17
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	4	0.17
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	4	0.17
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	14	0.17
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	14	0.17
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	14	0.17
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	14	0.17
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	14	0.17
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	14	0.17
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	13	0.17
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	13	0.17
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	9	0.17
(2,422)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	9	0.17
(2,422)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	9	0.17
(2,422)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	9	0.17
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	9	0.17
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	9	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	9	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	9	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	9	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	9	0.17
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	10	0.17
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	10	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	10	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	10	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	10	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	15	0.17
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	15	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	15	0.17
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	15	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	15	0.17
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	15	0.17
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	6	0.17
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	6	0.17
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.17
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.17
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.17
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.17
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.17
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.17
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	13	0.17
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	13	0.17
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	13	0.17
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	13	0.17
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	13	0.17
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	13	0.17
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.17
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.17
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.17
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.17
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.17
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.17
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.17
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.17
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.17
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.17
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.17
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.17
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.17
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.17
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.17
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.17
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.17
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	3	0.17
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	3	0.17
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	3	0.17
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	15	0.17
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	15	0.17
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.17
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.17
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.17
(2,140)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.17
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.17
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.17
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.17
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.17
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.17
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.17
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.17
(2,1338)	1:786:A:GLY:H	1:782:A:VAL:HA	13	0.16
(2,1294)	1:778:A:VAL:HG21	1:775:A:LEU:HA	4	0.16
(2,1294)	1:778:A:VAL:HG22	1:775:A:LEU:HA	4	0.16
(2,1294)	1:778:A:VAL:HG23	1:775:A:LEU:HA	4	0.16
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	1	0.16
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	1	0.16
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	1	0.16
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	14	0.16
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	14	0.16
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	14	0.16
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	3	0.16
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	3	0.16
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	3	0.16
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	3	0.16
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	3	0.16
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	3	0.16
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	4	0.16
(2,1239)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	4	0.16
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	1	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	3	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	3	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	3	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	3	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	3	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	4	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	4	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	4	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	4	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	4	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	4	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	5	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	5	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	5	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	5	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	5	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	5	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	8	0.16
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	8	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	8	0.16
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	8	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	8	0.16
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	8	0.16
(2,1209)	1:749:A:VAL:H	1:746:A:ILE:HA	9	0.16
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	3	0.16
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	3	0.16
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	2	0.16
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	2	0.16
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	2	0.16
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	2	0.16
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	2	0.16
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	2	0.16
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	13	0.16
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	13	0.16
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	13	0.16
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	13	0.16
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	13	0.16
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	13	0.16
(2,1150)	1:708:A:VAL:H	1:705:A:VAL:HA	14	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG2	7	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG3	7	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG2	14	0.16
(2,1147)	1:707:A:ARG:H	1:707:A:ARG:HG3	14	0.16
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.16
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.16
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.16
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.16
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.16
(2,1090)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.16
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	3	0.16
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	3	0.16
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	3	0.16
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	3	0.16
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	3	0.16
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	3	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.16
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.16
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.16
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.16
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.16
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.16
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.16
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.16
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.16
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.16
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.16
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.16
(2,1012)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.16
(2,1008)	1:676:A:THR:HG21	1:681:A:TYR:HH	13	0.16
(2,1008)	1:676:A:THR:HG22	1:681:A:TYR:HH	13	0.16
(2,1008)	1:676:A:THR:HG23	1:681:A:TYR:HH	13	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	5	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	5	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	5	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	5	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	5	0.16
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	5	0.16
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	5	0.16
(2,932)	1:786:A:GLY:H	1:782:A:VAL:HA	13	0.16
(2,888)	1:778:A:VAL:HG21	1:775:A:LEU:HA	4	0.16
(2,888)	1:778:A:VAL:HG22	1:775:A:LEU:HA	4	0.16
(2,888)	1:778:A:VAL:HG23	1:775:A:LEU:HA	4	0.16
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	1	0.16
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	1	0.16
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	1	0.16
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	14	0.16
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	14	0.16
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	14	0.16
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	3	0.16
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	3	0.16
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	3	0.16
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	3	0.16
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	3	0.16
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	3	0.16
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	4	0.16
(2,833)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	4	0.16
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	1	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	3	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	3	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	3	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	3	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	3	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	3	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	4	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	4	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	4	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	4	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	4	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	5	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	5	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	5	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	5	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	5	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	5	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	8	0.16
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	8	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	8	0.16
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	8	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	8	0.16
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	8	0.16
(2,803)	1:749:A:VAL:H	1:746:A:ILE:HA	9	0.16
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	3	0.16
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	3	0.16
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	2	0.16
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	2	0.16
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	2	0.16
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	2	0.16
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	2	0.16
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	2	0.16
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	13	0.16
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	13	0.16
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	13	0.16
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	13	0.16
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	13	0.16
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	13	0.16
(2,744)	1:708:A:VAL:H	1:705:A:VAL:HA	14	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG2	7	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG3	7	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG2	14	0.16
(2,741)	1:707:A:ARG:H	1:707:A:ARG:HG3	14	0.16
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.16
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.16
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.16
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.16
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.16
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.16
(2,684)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	3	0.16
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	3	0.16
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	3	0.16
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	3	0.16
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	3	0.16
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	3	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.16
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.16
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.16
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.16
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.16
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.16
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.16
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.16
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.16
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.16
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.16
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.16
(2,606)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.16
(2,602)	1:676:A:THR:HG21	1:681:A:TYR:HH	13	0.16
(2,602)	1:676:A:THR:HG22	1:681:A:TYR:HH	13	0.16
(2,602)	1:676:A:THR:HG23	1:681:A:TYR:HH	13	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	5	0.16
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	5	0.16
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	5	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	5	0.16
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	5	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	5	0.16
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	5	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	5	0.16
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	5	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	5	0.16
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	5	0.16
(2,526)	1:786:A:GLY:H	1:782:A:VAL:HA	13	0.16
(2,482)	1:778:A:VAL:HG21	1:775:A:LEU:HA	4	0.16
(2,482)	1:778:A:VAL:HG22	1:775:A:LEU:HA	4	0.16
(2,482)	1:778:A:VAL:HG23	1:775:A:LEU:HA	4	0.16
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	1	0.16
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	1	0.16
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	1	0.16
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	14	0.16
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	14	0.16
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	14	0.16
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	3	0.16
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	3	0.16
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	3	0.16
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	3	0.16
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	3	0.16
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	3	0.16
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD2	4	0.16
(2,427)	1:757:A:TRP:HE1	1:761:A:ARG:HD3	4	0.16
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	1	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	3	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	3	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	3	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	3	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	3	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	3	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	4	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	4	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	4	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	4	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	4	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	4	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	5	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	5	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	5	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	5	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	5	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	8	0.16
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	8	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	8	0.16
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	8	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	8	0.16
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	8	0.16
(2,397)	1:749:A:VAL:H	1:746:A:ILE:HA	9	0.16
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	3	0.16
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	3	0.16
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	10	0.16
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	2	0.16
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	2	0.16
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	2	0.16
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	2	0.16
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	2	0.16
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	2	0.16
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	13	0.16
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	13	0.16
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	13	0.16
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	13	0.16
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	13	0.16
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	13	0.16
(2,338)	1:708:A:VAL:H	1:705:A:VAL:HA	14	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG2	7	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG3	7	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG2	14	0.16
(2,335)	1:707:A:ARG:H	1:707:A:ARG:HG3	14	0.16
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.16
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.16
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.16
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.16
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.16
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.16
(2,278)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.16
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	3	0.16
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	3	0.16
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	3	0.16
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	3	0.16
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	3	0.16
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.16
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.16
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.16
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.16
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.16
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.16
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.16
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.16
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.16
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.16
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.16
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.16
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.16
(2,200)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.16
(2,196)	1:676:A:THR:HG21	1:681:A:TYR:HH	13	0.16
(2,196)	1:676:A:THR:HG22	1:681:A:TYR:HH	13	0.16
(2,196)	1:676:A:THR:HG23	1:681:A:TYR:HH	13	0.16
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.16
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	5	0.16
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	5	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	5	0.16
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	5	0.16
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	5	0.16
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	5	0.16
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	5	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	5	0.16
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	5	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	5	0.16
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	5	0.16
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB2	11	0.16
(2,6)	1:663:A:LEU:H	1:661:A:LEU:HB3	11	0.16
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB2	11	0.16
(2,5)	1:663:A:LEU:H	1:661:A:LEU:HB3	11	0.16
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB2	11	0.16
(2,4)	1:663:A:LEU:H	1:661:A:LEU:HB3	11	0.16
(1,69)	1:753:C:LEU:O	1:757:C:TRP:H	13	0.16
(1,43)	1:753:C:LEU:O	1:757:C:TRP:H	13	0.16
(1,17)	1:753:C:LEU:O	1:757:C:TRP:H	13	0.16
(2,1347)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	13	0.15
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	5	0.15
(2,1329)	1:784:A:LEU:HD11	1:787:A:ARG:HD2	5	0.15
(2,1329)	1:784:A:LEU:HD11	1:787:A:ARG:HD3	5	0.15
(2,1329)	1:784:A:LEU:HD12	1:787:A:ARG:HD2	5	0.15
(2,1329)	1:784:A:LEU:HD12	1:787:A:ARG:HD3	5	0.15
(2,1329)	1:784:A:LEU:HD13	1:787:A:ARG:HD2	5	0.15
(2,1329)	1:784:A:LEU:HD13	1:787:A:ARG:HD3	5	0.15
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	6	0.15
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	6	0.15
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	3	0.15
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	7	0.15
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	7	0.15
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	7	0.15
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	7	0.15
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	7	0.15
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	7	0.15
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	11	0.15
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	11	0.15
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	11	0.15
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	11	0.15
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	11	0.15
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	11	0.15
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	3	0.15
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	10	0.15
(2,1256)	1:771:A:LEU:HD11	1:764:A:SER:HA	12	0.15
(2,1256)	1:771:A:LEU:HD12	1:764:A:SER:HA	12	0.15
(2,1256)	1:771:A:LEU:HD13	1:764:A:SER:HA	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	12	0.15
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	15	0.15
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	15	0.15
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	15	0.15
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	15	0.15
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	15	0.15
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	15	0.15
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	12	0.15
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	12	0.15
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	13	0.15
(2,1234)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	15	0.15
(2,1234)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	15	0.15
(2,1234)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	15	0.15
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	14	0.15
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	14	0.15
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	14	0.15
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	14	0.15
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	14	0.15
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	14	0.15
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	13	0.15
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	13	0.15
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	13	0.15
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	13	0.15
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	13	0.15
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	13	0.15
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	2	0.15
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	10	0.15
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	15	0.15
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	6	0.15
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.15
(2,1150)	1:708:A:VAL:H	1:705:A:VAL:HA	5	0.15
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	6	0.15
(2,1120)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	6	0.15
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	6	0.15
(2,1120)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	6	0.15
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	6	0.15
(2,1120)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	6	0.15
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.15
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.15
(2,1101)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.15
(2,1096)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.15
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.15
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.15
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.15
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.15
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.15
(2,1083)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.15
(2,1083)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.15
(2,1083)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.15
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	2	0.15
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	2	0.15
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	2	0.15
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	2	0.15
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	2	0.15
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	2	0.15
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.15
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.15
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.15
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	1	0.15
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	1	0.15
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	1	0.15
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.15
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.15
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.15
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.15
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.15
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.15
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	6	0.15
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	6	0.15
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	6	0.15
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15
(2,1000)	1:674:A:ASP:H	1:677:A:ASN:H	15	0.15
(2,981)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.15
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.15
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.15
(2,941)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	13	0.15
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	5	0.15
(2,923)	1:784:A:LEU:HD11	1:787:A:ARG:HD2	5	0.15
(2,923)	1:784:A:LEU:HD11	1:787:A:ARG:HD3	5	0.15
(2,923)	1:784:A:LEU:HD12	1:787:A:ARG:HD2	5	0.15
(2,923)	1:784:A:LEU:HD12	1:787:A:ARG:HD3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,923)	1:784:A:LEU:HD13	1:787:A:ARG:HD2	5	0.15
(2,923)	1:784:A:LEU:HD13	1:787:A:ARG:HD3	5	0.15
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	6	0.15
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	6	0.15
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	3	0.15
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	7	0.15
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	7	0.15
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	7	0.15
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	7	0.15
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	7	0.15
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	7	0.15
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	11	0.15
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	11	0.15
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	11	0.15
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	11	0.15
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	11	0.15
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	11	0.15
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	3	0.15
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	10	0.15
(2,850)	1:771:A:LEU:HD11	1:764:A:SER:HA	12	0.15
(2,850)	1:771:A:LEU:HD12	1:764:A:SER:HA	12	0.15
(2,850)	1:771:A:LEU:HD13	1:764:A:SER:HA	12	0.15
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	12	0.15
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	15	0.15
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	15	0.15
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	15	0.15
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	15	0.15
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	15	0.15
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	15	0.15
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	12	0.15
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	12	0.15
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	13	0.15
(2,828)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	15	0.15
(2,828)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	15	0.15
(2,828)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	15	0.15
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	14	0.15
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	14	0.15
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	14	0.15
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	14	0.15
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	14	0.15
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	14	0.15
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	13	0.15
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	13	0.15
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	13	0.15
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	13	0.15
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	13	0.15
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	2	0.15
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	10	0.15
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	15	0.15
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	6	0.15
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.15
(2,744)	1:708:A:VAL:H	1:705:A:VAL:HA	5	0.15
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	6	0.15
(2,714)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	6	0.15
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	6	0.15
(2,714)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	6	0.15
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	6	0.15
(2,714)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	6	0.15
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.15
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.15
(2,695)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.15
(2,690)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.15
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.15
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.15
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.15
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.15
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.15
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.15
(2,677)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.15
(2,677)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.15
(2,677)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.15
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	2	0.15
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	2	0.15
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	2	0.15
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	2	0.15
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	2	0.15
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	2	0.15
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.15
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.15
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.15
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	1	0.15
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	1	0.15
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.15
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.15
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.15
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.15
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.15
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.15
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	6	0.15
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	6	0.15
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	6	0.15
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15
(2,594)	1:674:A:ASP:H	1:677:A:ASN:H	15	0.15
(2,575)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.15
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.15
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.15
(2,535)	1:780:A:ARG:HH11	1:783:A:GLU:OE1	13	0.15
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	5	0.15
(2,517)	1:784:A:LEU:HD11	1:787:A:ARG:HD2	5	0.15
(2,517)	1:784:A:LEU:HD11	1:787:A:ARG:HD3	5	0.15
(2,517)	1:784:A:LEU:HD12	1:787:A:ARG:HD2	5	0.15
(2,517)	1:784:A:LEU:HD12	1:787:A:ARG:HD3	5	0.15
(2,517)	1:784:A:LEU:HD13	1:787:A:ARG:HD2	5	0.15
(2,517)	1:784:A:LEU:HD13	1:787:A:ARG:HD3	5	0.15
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	6	0.15
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	6	0.15
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	3	0.15
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	7	0.15
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	7	0.15
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	7	0.15
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	7	0.15
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	7	0.15
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	7	0.15
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	11	0.15
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	11	0.15
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	11	0.15
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	11	0.15
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	11	0.15
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	11	0.15
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	3	0.15
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	10	0.15
(2,444)	1:771:A:LEU:HD11	1:764:A:SER:HA	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,444)	1:771:A:LEU:HD12	1:764:A:SER:HA	12	0.15
(2,444)	1:771:A:LEU:HD13	1:764:A:SER:HA	12	0.15
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	12	0.15
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	15	0.15
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	15	0.15
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	15	0.15
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	15	0.15
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	15	0.15
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	15	0.15
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	12	0.15
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	12	0.15
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	13	0.15
(2,422)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	15	0.15
(2,422)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	15	0.15
(2,422)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	15	0.15
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	14	0.15
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	14	0.15
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	14	0.15
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	14	0.15
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	14	0.15
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	14	0.15
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	13	0.15
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	13	0.15
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	13	0.15
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	13	0.15
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	13	0.15
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	13	0.15
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	2	0.15
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	10	0.15
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	15	0.15
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	6	0.15
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	8	0.15
(2,338)	1:708:A:VAL:H	1:705:A:VAL:HA	5	0.15
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	6	0.15
(2,308)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	6	0.15
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	6	0.15
(2,308)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	6	0.15
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	6	0.15
(2,308)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	6	0.15
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.15
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.15
(2,289)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.15
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.15
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.15
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.15
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.15
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.15
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.15
(2,271)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.15
(2,271)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.15
(2,271)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.15
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	2	0.15
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	2	0.15
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	2	0.15
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	2	0.15
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	2	0.15
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	2	0.15
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.15
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.15
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.15
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	1	0.15
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	1	0.15
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	1	0.15
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.15
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.15
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.15
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.15
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.15
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.15
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	6	0.15
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	6	0.15
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	6	0.15
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.15
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.15
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.15
(2,188)	1:674:A:ASP:H	1:677:A:ASN:H	15	0.15
(2,169)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.15
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.15
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.15
(1,75)	1:756:C:ILE:O	1:760:C:LEU:H	15	0.15
(1,49)	1:756:C:ILE:O	1:760:C:LEU:H	15	0.15
(1,23)	1:756:C:ILE:O	1:760:C:LEU:H	15	0.15
(2,1331)	1:785:A:LEU:H	1:782:A:VAL:HA	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD2	4	0.14
(2,1318)	1:783:A:GLU:H	1:780:A:ARG:HD3	4	0.14
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	14	0.14
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.14
(2,1252)	1:763:A:LEU:HD21	1:771:A:LEU:HB2	5	0.14
(2,1252)	1:763:A:LEU:HD21	1:771:A:LEU:HB3	5	0.14
(2,1252)	1:763:A:LEU:HD22	1:771:A:LEU:HB2	5	0.14
(2,1252)	1:763:A:LEU:HD22	1:771:A:LEU:HB3	5	0.14
(2,1252)	1:763:A:LEU:HD23	1:771:A:LEU:HB2	5	0.14
(2,1252)	1:763:A:LEU:HD23	1:771:A:LEU:HB3	5	0.14
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	13	0.14
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	13	0.14
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	13	0.14
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	13	0.14
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	13	0.14
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	13	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	4	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	4	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	4	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	4	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	4	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	4	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	14	0.14
(2,1245)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	14	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	14	0.14
(2,1245)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	14	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	14	0.14
(2,1245)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	14	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	5	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	5	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	7	0.14
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	7	0.14
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	15	0.14
(2,1234)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	13	0.14
(2,1234)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	13	0.14
(2,1234)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	13	0.14
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	6	0.14
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	6	0.14
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	6	0.14
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	6	0.14
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	6	0.14
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB2	15	0.14
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB3	15	0.14
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB2	13	0.14
(2,1157)	1:708:A:VAL:HG21	1:745:A:SER:HB3	13	0.14
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB2	13	0.14
(2,1157)	1:708:A:VAL:HG22	1:745:A:SER:HB3	13	0.14
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB2	13	0.14
(2,1157)	1:708:A:VAL:HG23	1:745:A:SER:HB3	13	0.14
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	12	0.14
(2,1156)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	12	0.14
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	12	0.14
(2,1156)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	12	0.14
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	12	0.14
(2,1156)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	12	0.14
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.14
(2,1148)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.14
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.14
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.14
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.14
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.14
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.14
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.14
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.14
(2,1067)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.14
(2,1067)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.14
(2,1067)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.14
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.14
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.14
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.14
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.14
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.14
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.14
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	0.14
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	0.14
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	0.14
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	0.14
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	0.14
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	0.14
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	0.14
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	0.14
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	0.14
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.14
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.14
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.14
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.14
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.14
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.14
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.14
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.14
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.14
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.14
(2,925)	1:785:A:LEU:H	1:782:A:VAL:HA	8	0.14
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD2	4	0.14
(2,912)	1:783:A:GLU:H	1:780:A:ARG:HD3	4	0.14
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	14	0.14
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.14
(2,846)	1:763:A:LEU:HD21	1:771:A:LEU:HB2	5	0.14
(2,846)	1:763:A:LEU:HD21	1:771:A:LEU:HB3	5	0.14
(2,846)	1:763:A:LEU:HD22	1:771:A:LEU:HB2	5	0.14
(2,846)	1:763:A:LEU:HD22	1:771:A:LEU:HB3	5	0.14
(2,846)	1:763:A:LEU:HD23	1:771:A:LEU:HB2	5	0.14
(2,846)	1:763:A:LEU:HD23	1:771:A:LEU:HB3	5	0.14
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	13	0.14
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	13	0.14
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	13	0.14
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	13	0.14
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	13	0.14
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	13	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	4	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	4	0.14
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	4	0.14
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	4	0.14
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	4	0.14
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	4	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	14	0.14
(2,839)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	14	0.14
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	14	0.14
(2,839)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	14	0.14
(2,839)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	14	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	5	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	5	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	7	0.14
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	7	0.14
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	15	0.14
(2,828)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	13	0.14
(2,828)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	13	0.14
(2,828)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	13	0.14
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	6	0.14
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	6	0.14
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	6	0.14
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	6	0.14
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	6	0.14
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	6	0.14
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB2	15	0.14
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB3	15	0.14
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB2	13	0.14
(2,751)	1:708:A:VAL:HG21	1:745:A:SER:HB3	13	0.14
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB2	13	0.14
(2,751)	1:708:A:VAL:HG22	1:745:A:SER:HB3	13	0.14
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB2	13	0.14
(2,751)	1:708:A:VAL:HG23	1:745:A:SER:HB3	13	0.14
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	12	0.14
(2,750)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	12	0.14
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	12	0.14
(2,750)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	12	0.14
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	12	0.14
(2,750)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	12	0.14
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.14
(2,742)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.14
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.14
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.14
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.14
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.14
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.14
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.14
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.14
(2,661)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.14
(2,661)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.14
(2,661)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.14
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.14
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.14
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.14
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.14
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.14
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	0.14
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	0.14
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	0.14
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	0.14
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	0.14
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	0.14
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	0.14
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	0.14
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	0.14
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.14
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.14
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.14
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.14
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.14
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.14
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.14
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.14
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.14
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.14
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.14
(2,519)	1:785:A:LEU:H	1:782:A:VAL:HA	8	0.14
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD2	4	0.14
(2,506)	1:783:A:GLU:H	1:780:A:ARG:HD3	4	0.14
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	14	0.14
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	7	0.14
(2,440)	1:763:A:LEU:HD21	1:771:A:LEU:HB2	5	0.14
(2,440)	1:763:A:LEU:HD21	1:771:A:LEU:HB3	5	0.14
(2,440)	1:763:A:LEU:HD22	1:771:A:LEU:HB2	5	0.14
(2,440)	1:763:A:LEU:HD22	1:771:A:LEU:HB3	5	0.14
(2,440)	1:763:A:LEU:HD23	1:771:A:LEU:HB2	5	0.14
(2,440)	1:763:A:LEU:HD23	1:771:A:LEU:HB3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	13	0.14
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	13	0.14
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	13	0.14
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	13	0.14
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	13	0.14
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	13	0.14
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	4	0.14
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	4	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	4	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	4	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	4	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	4	0.14
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG12	14	0.14
(2,433)	1:760:A:LEU:HD11	1:756:A:ILE:HG13	14	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG12	14	0.14
(2,433)	1:760:A:LEU:HD12	1:756:A:ILE:HG13	14	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG12	14	0.14
(2,433)	1:760:A:LEU:HD13	1:756:A:ILE:HG13	14	0.14
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	5	0.14
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	5	0.14
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	7	0.14
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	7	0.14
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	15	0.14
(2,422)	1:755:A:LEU:HD21	1:759:A:ASP:HB3	13	0.14
(2,422)	1:755:A:LEU:HD22	1:759:A:ASP:HB3	13	0.14
(2,422)	1:755:A:LEU:HD23	1:759:A:ASP:HB3	13	0.14
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	6	0.14
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	6	0.14
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	6	0.14
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	6	0.14
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	6	0.14
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	6	0.14
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB2	15	0.14
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB3	15	0.14
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB2	13	0.14
(2,345)	1:708:A:VAL:HG21	1:745:A:SER:HB3	13	0.14
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB2	13	0.14
(2,345)	1:708:A:VAL:HG22	1:745:A:SER:HB3	13	0.14
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB2	13	0.14
(2,345)	1:708:A:VAL:HG23	1:745:A:SER:HB3	13	0.14
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD2	12	0.14
(2,344)	1:708:A:VAL:HG21	1:707:A:ARG:HD3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD2	12	0.14
(2,344)	1:708:A:VAL:HG22	1:707:A:ARG:HD3	12	0.14
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD2	12	0.14
(2,344)	1:708:A:VAL:HG23	1:707:A:ARG:HD3	12	0.14
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.14
(2,336)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.14
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.14
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.14
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.14
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.14
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.14
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.14
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.14
(2,255)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.14
(2,255)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.14
(2,255)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.14
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.14
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.14
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.14
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.14
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.14
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.14
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	0.14
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	0.14
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	0.14
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	0.14
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	0.14
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	0.14
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	0.14
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	0.14
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	0.14
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.14
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.14
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.14
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.14
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.14
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.14
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.14
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.14
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.14
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.14
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.14
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.14
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.14
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.14
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.14
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	12	0.14
(2,63)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	12	0.14
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	12	0.14
(2,63)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	12	0.14
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	12	0.14
(2,63)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	12	0.14
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	12	0.14
(2,62)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	12	0.14
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	12	0.14
(2,62)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	12	0.14
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	12	0.14
(2,62)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	12	0.14
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB2	12	0.14
(2,61)	1:700:A:ALA:HB1	1:702:A:LEU:HB3	12	0.14
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB2	12	0.14
(2,61)	1:700:A:ALA:HB2	1:702:A:LEU:HB3	12	0.14
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB2	12	0.14
(2,61)	1:700:A:ALA:HB3	1:702:A:LEU:HB3	12	0.14
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.14
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.14
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.14
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.14
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.14
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.14
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.14
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.14
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.14
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.14
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.14
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.14
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.14
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.14
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.14
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.14
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.14
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.14
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.14
(2,54)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.14
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.14
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.14
(2,53)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.14
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.14
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.14
(2,52)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.14
(1,56)	1:741:C:ASP:O	1:745:C:SER:N	13	0.14
(1,30)	1:741:C:ASP:O	1:745:C:SER:N	13	0.14
(1,4)	1:741:C:ASP:O	1:745:C:SER:N	13	0.14
(2,1343)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	10	0.13
(2,1336)	1:785:A:LEU:H	1:787:A:ARG:H	5	0.13
(2,1305)	1:781:A:ILE:H	1:778:A:VAL:HA	14	0.13
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	9	0.13
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	9	0.13
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	9	0.13
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	9	0.13
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	9	0.13
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	9	0.13
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	4	0.13
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	11	0.13
(2,1243)	1:759:A:ASP:H	1:759:A:ASP:HB3	13	0.13
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	2	0.13
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	2	0.13
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	2	0.13
(2,1229)	1:755:A:LEU:H	1:752:A:SER:HA	8	0.13
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	11	0.13
(2,1225)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	11	0.13
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	11	0.13
(2,1225)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	11	0.13
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	11	0.13
(2,1225)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	11	0.13
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	11	0.13
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	11	0.13
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	7	0.13
(2,1155)	1:708:A:VAL:HG11	1:705:A:VAL:HA	4	0.13
(2,1155)	1:708:A:VAL:HG12	1:705:A:VAL:HA	4	0.13
(2,1155)	1:708:A:VAL:HG13	1:705:A:VAL:HA	4	0.13
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	9	0.13
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	9	0.13
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.13
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.13
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.13
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.13
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.13
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.13
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.13
(2,1121)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.13
(2,1121)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.13
(2,1121)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.13
(2,1121)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.13
(2,1121)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.13
(2,1121)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.13
(2,1094)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.13
(2,1094)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.13
(2,1094)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.13
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.13
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.13
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.13
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	14	0.13
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	14	0.13
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	14	0.13
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	14	0.13
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	14	0.13
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	14	0.13
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	15	0.13
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	15	0.13
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	15	0.13
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	15	0.13
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	15	0.13
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	15	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	1	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	1	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	1	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	1	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	1	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.13
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.13
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.13
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.13
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	11	0.13
(2,1054)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	11	0.13
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	11	0.13
(2,1054)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	11	0.13
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	11	0.13
(2,1054)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	11	0.13
(2,1047)	1:686:A:ILE:HD11	1:685:A:PHE:HD1	15	0.13
(2,1047)	1:686:A:ILE:HD11	1:685:A:PHE:HD2	15	0.13
(2,1047)	1:686:A:ILE:HD12	1:685:A:PHE:HD1	15	0.13
(2,1047)	1:686:A:ILE:HD12	1:685:A:PHE:HD2	15	0.13
(2,1047)	1:686:A:ILE:HD13	1:685:A:PHE:HD1	15	0.13
(2,1047)	1:686:A:ILE:HD13	1:685:A:PHE:HD2	15	0.13
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.13
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.13
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.13
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.13
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.13
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.13
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.13
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.13
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.13
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.13
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.13
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.13
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.13
(2,950)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.13
(2,950)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.13
(2,950)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.13
(2,950)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.13
(2,950)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.13
(2,950)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.13
(2,950)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.13
(2,950)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.13
(2,950)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.13
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.13
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.13
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.13
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.13
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.13
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.13
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.13
(2,937)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	10	0.13
(2,930)	1:785:A:LEU:H	1:787:A:ARG:H	5	0.13
(2,899)	1:781:A:ILE:H	1:778:A:VAL:HA	14	0.13
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	9	0.13
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	9	0.13
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	9	0.13
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	9	0.13
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	9	0.13
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	9	0.13
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	4	0.13
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	11	0.13
(2,837)	1:759:A:ASP:H	1:759:A:ASP:HB3	13	0.13
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	2	0.13
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	2	0.13
(2,823)	1:755:A:LEU:H	1:752:A:SER:HA	8	0.13
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	11	0.13
(2,819)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	11	0.13
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	11	0.13
(2,819)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	11	0.13
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	11	0.13
(2,819)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	11	0.13
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	11	0.13
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	11	0.13
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	7	0.13
(2,749)	1:708:A:VAL:HG11	1:705:A:VAL:HA	4	0.13
(2,749)	1:708:A:VAL:HG12	1:705:A:VAL:HA	4	0.13
(2,749)	1:708:A:VAL:HG13	1:705:A:VAL:HA	4	0.13
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	9	0.13
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	9	0.13
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.13
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.13
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.13
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.13
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.13
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.13
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.13
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.13
(2,715)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.13
(2,715)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.13
(2,715)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.13
(2,715)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.13
(2,715)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.13
(2,715)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.13
(2,688)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.13
(2,688)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.13
(2,688)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.13
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.13
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.13
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.13
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.13
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.13
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	14	0.13
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	14	0.13
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	14	0.13
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	14	0.13
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	14	0.13
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	14	0.13
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	15	0.13
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	15	0.13
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	15	0.13
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	15	0.13
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	15	0.13
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	15	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	1	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	1	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	1	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	1	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	1	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	1	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.13
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.13
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.13
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.13
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	11	0.13
(2,648)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	11	0.13
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	11	0.13
(2,648)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	11	0.13
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	11	0.13
(2,648)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	11	0.13
(2,641)	1:686:A:ILE:HD11	1:685:A:PHE:HD1	15	0.13
(2,641)	1:686:A:ILE:HD11	1:685:A:PHE:HD2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:686:A:ILE:HD12	1:685:A:PHE:HD1	15	0.13
(2,641)	1:686:A:ILE:HD12	1:685:A:PHE:HD2	15	0.13
(2,641)	1:686:A:ILE:HD13	1:685:A:PHE:HD1	15	0.13
(2,641)	1:686:A:ILE:HD13	1:685:A:PHE:HD2	15	0.13
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.13
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.13
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.13
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.13
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.13
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.13
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.13
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.13
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.13
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.13
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.13
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.13
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.13
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.13
(2,544)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.13
(2,544)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.13
(2,544)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.13
(2,544)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.13
(2,544)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.13
(2,544)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.13
(2,544)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.13
(2,544)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.13
(2,544)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.13
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.13
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.13
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.13
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.13
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.13
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.13
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.13
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.13
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.13
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.13
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.13
(2,531)	1:740:A:ARG:HH21	1:743:A:ASP:OD2	10	0.13
(2,524)	1:785:A:LEU:H	1:787:A:ARG:H	5	0.13
(2,493)	1:781:A:ILE:H	1:778:A:VAL:HA	14	0.13
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	9	0.13
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	9	0.13
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	9	0.13
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	9	0.13
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	9	0.13
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	9	0.13
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	4	0.13
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	11	0.13
(2,431)	1:759:A:ASP:H	1:759:A:ASP:HB3	13	0.13
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	2	0.13
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	2	0.13
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	2	0.13
(2,417)	1:755:A:LEU:H	1:752:A:SER:HA	8	0.13
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA2	11	0.13
(2,413)	1:754:A:ALA:HB1	1:751:A:GLY:HA3	11	0.13
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA2	11	0.13
(2,413)	1:754:A:ALA:HB2	1:751:A:GLY:HA3	11	0.13
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA2	11	0.13
(2,413)	1:754:A:ALA:HB3	1:751:A:GLY:HA3	11	0.13
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	11	0.13
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	11	0.13
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	7	0.13
(2,343)	1:708:A:VAL:HG11	1:705:A:VAL:HA	4	0.13
(2,343)	1:708:A:VAL:HG12	1:705:A:VAL:HA	4	0.13
(2,343)	1:708:A:VAL:HG13	1:705:A:VAL:HA	4	0.13
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	9	0.13
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	9	0.13
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.13
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.13
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.13
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.13
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.13
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.13
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.13
(2,309)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.13
(2,309)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.13
(2,309)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.13
(2,309)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.13
(2,309)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.13
(2,309)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.13
(2,282)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.13
(2,282)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.13
(2,282)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.13
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.13
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.13
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.13
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.13
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.13
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.13
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	14	0.13
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	14	0.13
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	14	0.13
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	14	0.13
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	14	0.13
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	14	0.13
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	15	0.13
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	15	0.13
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	15	0.13
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	15	0.13
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	15	0.13
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	15	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	1	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	1	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	1	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	1	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	1	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	1	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.13
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.13
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.13
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.13
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	11	0.13
(2,242)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	11	0.13
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	11	0.13
(2,242)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	11	0.13
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	11	0.13
(2,242)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	11	0.13
(2,235)	1:686:A:ILE:HD11	1:685:A:PHE:HD1	15	0.13
(2,235)	1:686:A:ILE:HD11	1:685:A:PHE:HD2	15	0.13
(2,235)	1:686:A:ILE:HD12	1:685:A:PHE:HD1	15	0.13
(2,235)	1:686:A:ILE:HD12	1:685:A:PHE:HD2	15	0.13
(2,235)	1:686:A:ILE:HD13	1:685:A:PHE:HD1	15	0.13
(2,235)	1:686:A:ILE:HD13	1:685:A:PHE:HD2	15	0.13
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.13
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.13
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.13
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.13
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.13
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.13
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.13
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.13
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.13
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.13
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.13
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.13
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.13
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.13
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.13
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.13
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.13
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.13
(2,138)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.13
(2,138)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.13
(2,138)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.13
(2,138)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.13
(2,138)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.13
(2,138)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.13
(2,138)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.13
(2,138)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.13
(2,138)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.13
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.13
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.13
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.13
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.13
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.13
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.13
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.13
(1,57)	1:742:C:ARG:O	1:746:C:ILE:H	5	0.13
(1,55)	1:741:C:ASP:O	1:745:C:SER:H	11	0.13
(1,53)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.13
(1,31)	1:742:C:ARG:O	1:746:C:ILE:H	5	0.13
(1,29)	1:741:C:ASP:O	1:745:C:SER:H	11	0.13
(1,27)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.13
(1,5)	1:742:C:ARG:O	1:746:C:ILE:H	5	0.13
(1,3)	1:741:C:ASP:O	1:745:C:SER:H	11	0.13
(1,1)	1:740:C:ARG:O	1:744:C:ARG:H	15	0.13
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	2	0.12
(2,1343)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	9	0.12
(2,1338)	1:786:A:GLY:H	1:782:A:VAL:HA	9	0.12
(2,1325)	1:784:A:LEU:H	1:783:A:GLU:HA	7	0.12
(2,1276)	1:776:A:LEU:H	1:773:A:ASP:HA	5	0.12
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	6	0.12
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	9	0.12
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	15	0.12
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	9	0.12
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	1	0.12
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	14	0.12
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	14	0.12
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	10	0.12
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	10	0.12
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	10	0.12
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	10	0.12
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	10	0.12
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	10	0.12
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	13	0.12
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	4	0.12
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	4	0.12
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	9	0.12
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	9	0.12
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	2	0.12
(2,1201)	1:747:A:ARG:H	1:744:A:ARG:HA	1	0.12
(2,1199)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	5	0.12
(2,1199)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	5	0.12
(2,1199)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	5	0.12
(2,1191)	1:746:A:ILE:H	1:743:A:ASP:HA	14	0.12
(2,1167)	1:710:A:GLN:H	1:709:A:ARG:HA	15	0.12
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.12
(2,1133)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.12
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.12
(2,1133)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.12
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.12
(2,1133)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.12
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.12
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.12
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.12
(2,1117)	1:704:A:LEU:H	1:704:A:LEU:HB3	2	0.12
(2,1101)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(2,1084)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	8	0.12
(2,1084)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	8	0.12
(2,1084)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	8	0.12
(2,1084)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1084)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	8	0.12
(2,1084)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	8	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.12
(2,1071)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.12
(2,1071)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.12
(2,1071)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.12
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	9	0.12
(2,1063)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	9	0.12
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	9	0.12
(2,1063)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	9	0.12
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	9	0.12
(2,1063)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	9	0.12
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	9	0.12
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	9	0.12
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	9	0.12
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	9	0.12
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	9	0.12
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	9	0.12
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.12
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.12
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.12
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.12
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.12
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.12
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.12
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.12
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.12
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.12
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.12
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.12
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.12
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.12
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.12
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.12
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.12
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.12
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.12
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.12
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.12
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.12
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.12
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.12
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.12
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.12
(2,1008)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.12
(2,1008)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.12
(2,1008)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.12
(2,1008)	1:676:A:THR:HG21	1:681:A:TYR:HH	9	0.12
(2,1008)	1:676:A:THR:HG22	1:681:A:TYR:HH	9	0.12
(2,1008)	1:676:A:THR:HG23	1:681:A:TYR:HH	9	0.12
(2,1008)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.12
(2,1008)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.12
(2,1008)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.12
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.12
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.12
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.12
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.12
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.12
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.12
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.12
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.12
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.12
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.12
(2,987)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.12
(2,987)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12
(2,986)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.12
(2,986)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.12
(2,986)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.12
(2,986)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.12
(2,986)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.12
(2,981)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.12
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.12
(2,962)	1:666:A:TRP:H	1:663:A:LEU:HA	2	0.12
(2,962)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.12
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.12
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.12
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.12
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.12
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.12
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.12
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.12
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	2	0.12
(2,937)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	9	0.12
(2,932)	1:786:A:GLY:H	1:782:A:VAL:HA	9	0.12
(2,919)	1:784:A:LEU:H	1:783:A:GLU:HA	7	0.12
(2,870)	1:776:A:LEU:H	1:773:A:ASP:HA	5	0.12
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	6	0.12
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	9	0.12
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	15	0.12
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	9	0.12
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	1	0.12
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	1	0.12
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	14	0.12
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	14	0.12
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	10	0.12
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	10	0.12
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	10	0.12
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	10	0.12
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	10	0.12
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	10	0.12
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	13	0.12
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	4	0.12
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	4	0.12
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	9	0.12
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	9	0.12
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,795)	1:747:A:ARG:H	1:744:A:ARG:HA	1	0.12
(2,793)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	5	0.12
(2,793)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	5	0.12
(2,793)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	5	0.12
(2,785)	1:746:A:ILE:H	1:743:A:ASP:HA	14	0.12
(2,761)	1:710:A:GLN:H	1:709:A:ARG:HA	15	0.12
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.12
(2,727)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.12
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.12
(2,727)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.12
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.12
(2,727)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.12
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.12
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.12
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.12
(2,711)	1:704:A:LEU:H	1:704:A:LEU:HB3	2	0.12
(2,695)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(2,678)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	8	0.12
(2,678)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	8	0.12
(2,678)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	8	0.12
(2,678)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	8	0.12
(2,678)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	8	0.12
(2,678)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	8	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.12
(2,665)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.12
(2,665)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.12
(2,665)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.12
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,657)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	9	0.12
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	9	0.12
(2,657)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	9	0.12
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	9	0.12
(2,657)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	9	0.12
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	9	0.12
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	9	0.12
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	9	0.12
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	9	0.12
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	9	0.12
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	9	0.12
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.12
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.12
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.12
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.12
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.12
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.12
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.12
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.12
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.12
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.12
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.12
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.12
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.12
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.12
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.12
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.12
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.12
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.12
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.12
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.12
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.12
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.12
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.12
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.12
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.12
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.12
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.12
(2,602)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.12
(2,602)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.12
(2,602)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.12
(2,602)	1:676:A:THR:HG21	1:681:A:TYR:HH	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,602)	1:676:A:THR:HG22	1:681:A:TYR:HH	9	0.12
(2,602)	1:676:A:THR:HG23	1:681:A:TYR:HH	9	0.12
(2,602)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.12
(2,602)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.12
(2,602)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.12
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.12
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.12
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.12
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.12
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.12
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.12
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.12
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.12
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.12
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.12
(2,581)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.12
(2,581)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12
(2,580)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.12
(2,580)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.12
(2,580)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.12
(2,580)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.12
(2,580)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.12
(2,580)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.12
(2,575)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.12
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.12
(2,556)	1:666:A:TRP:H	1:663:A:LEU:HA	2	0.12
(2,556)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.12
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.12
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.12
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.12
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.12
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.12
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.12
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	2	0.12
(2,531)	1:740:A:ARG:HH11	1:743:A:ASP:OD1	9	0.12
(2,526)	1:786:A:GLY:H	1:782:A:VAL:HA	9	0.12
(2,513)	1:784:A:LEU:H	1:783:A:GLU:HA	7	0.12
(2,464)	1:776:A:LEU:H	1:773:A:ASP:HA	5	0.12
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	6	0.12
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	9	0.12
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	15	0.12
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	9	0.12
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	1	0.12
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	1	0.12
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	14	0.12
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	14	0.12
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	10	0.12
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	10	0.12
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	10	0.12
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	10	0.12
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	10	0.12
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	10	0.12
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	13	0.12
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	4	0.12
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	4	0.12
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	9	0.12
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	9	0.12
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	2	0.12
(2,389)	1:747:A:ARG:H	1:744:A:ARG:HA	1	0.12
(2,387)	1:746:A:ILE:HG21	1:750:A:ASN:HD21	5	0.12
(2,387)	1:746:A:ILE:HG22	1:750:A:ASN:HD21	5	0.12
(2,387)	1:746:A:ILE:HG23	1:750:A:ASN:HD21	5	0.12
(2,379)	1:746:A:ILE:H	1:743:A:ASP:HA	14	0.12
(2,355)	1:710:A:GLN:H	1:709:A:ARG:HA	15	0.12
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.12
(2,321)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.12
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.12
(2,321)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.12
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.12
(2,321)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.12
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.12
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.12
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.12
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.12
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.12
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.12
(2,305)	1:704:A:LEU:H	1:704:A:LEU:HB3	2	0.12
(2,289)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(2,272)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	8	0.12
(2,272)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	8	0.12
(2,272)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	8	0.12
(2,272)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	8	0.12
(2,272)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	8	0.12
(2,272)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	8	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.12
(2,259)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.12
(2,259)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.12
(2,259)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.12
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	9	0.12
(2,251)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	9	0.12
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	9	0.12
(2,251)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	9	0.12
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	9	0.12
(2,251)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	9	0.12
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	9	0.12
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	9	0.12
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	9	0.12
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	9	0.12
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	9	0.12
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	9	0.12
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.12
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.12
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.12
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.12
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.12
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.12
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.12
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.12
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	3	0.12
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	3	0.12
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	3	0.12
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	3	0.12
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	3	0.12
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	3	0.12
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.12
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.12
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.12
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.12
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.12
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.12
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.12
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.12
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.12
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.12
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.12
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.12
(2,196)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.12
(2,196)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.12
(2,196)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.12
(2,196)	1:676:A:THR:HG21	1:681:A:TYR:HH	9	0.12
(2,196)	1:676:A:THR:HG22	1:681:A:TYR:HH	9	0.12
(2,196)	1:676:A:THR:HG23	1:681:A:TYR:HH	9	0.12
(2,196)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.12
(2,196)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.12
(2,196)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.12
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.12
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.12
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.12
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.12
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.12
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.12
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.12
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.12
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.12
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.12
(2,175)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.12
(2,175)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.12
(2,174)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.12
(2,174)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.12
(2,174)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.12
(2,174)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.12
(2,174)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.12
(2,174)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.12
(2,169)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.12
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.12
(2,150)	1:666:A:TRP:H	1:663:A:LEU:HA	2	0.12
(2,150)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.12
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.12
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.12
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.12
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.12
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.12
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.12
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.12
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.12
(2,60)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.12
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.12
(2,60)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.12
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.12
(2,60)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.12
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.12
(2,59)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.12
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.12
(2,59)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.12
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.12
(2,59)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.12
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.12
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.12
(2,58)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.12
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.12
(2,58)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.12
(2,1346)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	13	0.11
(2,1305)	1:781:A:ILE:H	1:778:A:VAL:HA	12	0.11
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	2	0.11
(2,1288)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	2	0.11
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	2	0.11
(2,1288)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	2	0.11
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	2	0.11
(2,1288)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	2	0.11
(2,1276)	1:776:A:LEU:H	1:773:A:ASP:HA	3	0.11
(2,1270)	1:775:A:LEU:H	1:772:A:ARG:HA	13	0.11
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	9	0.11
(2,1257)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	9	0.11
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	9	0.11
(2,1257)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	9	0.11
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	9	0.11
(2,1257)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	9	0.11
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	13	0.11
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	2	0.11
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	2	0.11
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	2	0.11
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	2	0.11
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	2	0.11
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	2	0.11
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	9	0.11
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	9	0.11
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	9	0.11
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	9	0.11
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	9	0.11
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	9	0.11
(2,1240)	1:758:A:ASP:H	1:754:A:ALA:HB1	7	0.11
(2,1240)	1:758:A:ASP:H	1:754:A:ALA:HB2	7	0.11
(2,1240)	1:758:A:ASP:H	1:754:A:ALA:HB3	7	0.11
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	8	0.11
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	8	0.11
(2,1227)	1:754:A:ALA:HB1	1:758:A:ASP:H	7	0.11
(2,1227)	1:754:A:ALA:HB2	1:758:A:ASP:H	7	0.11
(2,1227)	1:754:A:ALA:HB3	1:758:A:ASP:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	14	0.11
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	14	0.11
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	14	0.11
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	14	0.11
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	14	0.11
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	14	0.11
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	5	0.11
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	2	0.11
(2,1198)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	2	0.11
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	2	0.11
(2,1198)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	2	0.11
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	2	0.11
(2,1198)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	2	0.11
(2,1195)	1:746:A:ILE:H	1:747:A:ARG:H	9	0.11
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB2	8	0.11
(2,1192)	1:746:A:ILE:H	1:743:A:ASP:HB3	8	0.11
(2,1173)	1:710:A:GLN:HE21	1:706:A:ASN:HB2	6	0.11
(2,1173)	1:710:A:GLN:HE21	1:706:A:ASN:HB3	6	0.11
(2,1173)	1:710:A:GLN:HE22	1:706:A:ASN:HB2	6	0.11
(2,1173)	1:710:A:GLN:HE22	1:706:A:ASN:HB3	6	0.11
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	13	0.11
(2,1165)	1:709:A:ARG:HE	1:709:A:ARG:H	2	0.11
(2,1165)	1:709:A:ARG:HE	1:709:A:ARG:H	11	0.11
(2,1150)	1:708:A:VAL:H	1:705:A:VAL:HA	11	0.11
(2,1141)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.11
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.11
(2,1140)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.11
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.11
(2,1123)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.11
(2,1123)	1:705:A:VAL:H	1:702:A:LEU:HA	8	0.11
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	8	0.11
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	8	0.11
(2,1122)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	8	0.11
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	8	0.11
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	8	0.11
(2,1122)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	8	0.11
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	8	0.11
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	8	0.11
(2,1122)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	8	0.11
(2,1094)	1:700:A:ALA:HB1	1:697:A:ILE:HA	6	0.11
(2,1094)	1:700:A:ALA:HB2	1:697:A:ILE:HA	6	0.11
(2,1094)	1:700:A:ALA:HB3	1:697:A:ILE:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.11
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.11
(2,1081)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.11
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.11
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.11
(2,1081)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.11
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.11
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.11
(2,1081)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.11
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.11
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.11
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.11
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.11
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.11
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.11
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB2	12	0.11
(2,1060)	1:692:A:LEU:HD11	1:691:A:SER:HB3	12	0.11
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB2	12	0.11
(2,1060)	1:692:A:LEU:HD12	1:691:A:SER:HB3	12	0.11
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB2	12	0.11
(2,1060)	1:692:A:LEU:HD13	1:691:A:SER:HB3	12	0.11
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	6	0.11
(2,1055)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	6	0.11
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	6	0.11
(2,1055)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	6	0.11
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	6	0.11
(2,1055)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	6	0.11
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.11
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.11
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.11
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.11
(2,1051)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.11
(2,1051)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.11
(2,1051)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.11
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.11
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.11
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.11
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.11
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.11
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.11
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.11
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.11
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.11
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.11
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.11
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.11
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.11
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.11
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.11
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.11
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.11
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.11
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.11
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.11
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.11
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.11
(2,1025)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.11
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.11
(2,1025)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.11
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.11
(2,1025)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.11
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.11
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.11
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.11
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.11
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.11
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.11
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.11
(2,1014)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.11
(2,992)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.11
(2,987)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.11
(2,987)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(2,986)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(2,986)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(2,986)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(2,986)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(2,986)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11
(2,986)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(2,970)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.11
(2,962)	1:666:A:TRP:H	1:663:A:LEU:HA	13	0.11
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	0.11
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	0.11
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	0.11
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	0.11
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	0.11
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	0.11
(2,942)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	0.11
(2,940)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	13	0.11
(2,899)	1:781:A:ILE:H	1:778:A:VAL:HA	12	0.11
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	2	0.11
(2,882)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	2	0.11
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	2	0.11
(2,882)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	2	0.11
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	2	0.11
(2,882)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	2	0.11
(2,870)	1:776:A:LEU:H	1:773:A:ASP:HA	3	0.11
(2,864)	1:775:A:LEU:H	1:772:A:ARG:HA	13	0.11
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,851)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	9	0.11
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	9	0.11
(2,851)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	9	0.11
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	9	0.11
(2,851)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	9	0.11
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	13	0.11
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	2	0.11
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	2	0.11
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	2	0.11
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	2	0.11
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	2	0.11
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	2	0.11
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	9	0.11
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	9	0.11
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	9	0.11
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	9	0.11
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	9	0.11
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	9	0.11
(2,834)	1:758:A:ASP:H	1:754:A:ALA:HB1	7	0.11
(2,834)	1:758:A:ASP:H	1:754:A:ALA:HB2	7	0.11
(2,834)	1:758:A:ASP:H	1:754:A:ALA:HB3	7	0.11
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	8	0.11
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	8	0.11
(2,821)	1:754:A:ALA:HB1	1:758:A:ASP:H	7	0.11
(2,821)	1:754:A:ALA:HB2	1:758:A:ASP:H	7	0.11
(2,821)	1:754:A:ALA:HB3	1:758:A:ASP:H	7	0.11
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	14	0.11
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	14	0.11
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	14	0.11
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	14	0.11
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	14	0.11
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	14	0.11
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	5	0.11
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	2	0.11
(2,792)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	2	0.11
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	2	0.11
(2,792)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	2	0.11
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	2	0.11
(2,792)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	2	0.11
(2,789)	1:746:A:ILE:H	1:747:A:ARG:H	9	0.11
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB2	8	0.11
(2,786)	1:746:A:ILE:H	1:743:A:ASP:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,767)	1:710:A:GLN:HE21	1:706:A:ASN:HB2	6	0.11
(2,767)	1:710:A:GLN:HE21	1:706:A:ASN:HB3	6	0.11
(2,767)	1:710:A:GLN:HE22	1:706:A:ASN:HB2	6	0.11
(2,767)	1:710:A:GLN:HE22	1:706:A:ASN:HB3	6	0.11
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	13	0.11
(2,759)	1:709:A:ARG:HE	1:709:A:ARG:H	2	0.11
(2,759)	1:709:A:ARG:HE	1:709:A:ARG:H	11	0.11
(2,744)	1:708:A:VAL:H	1:705:A:VAL:HA	11	0.11
(2,735)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.11
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.11
(2,734)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.11
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.11
(2,717)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.11
(2,717)	1:705:A:VAL:H	1:702:A:LEU:HA	8	0.11
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	8	0.11
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	8	0.11
(2,716)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	8	0.11
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	8	0.11
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	8	0.11
(2,716)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	8	0.11
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	8	0.11
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	8	0.11
(2,716)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	8	0.11
(2,688)	1:700:A:ALA:HB1	1:697:A:ILE:HA	6	0.11
(2,688)	1:700:A:ALA:HB2	1:697:A:ILE:HA	6	0.11
(2,688)	1:700:A:ALA:HB3	1:697:A:ILE:HA	6	0.11
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.11
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.11
(2,675)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.11
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.11
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.11
(2,675)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.11
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.11
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.11
(2,675)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.11
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.11
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.11
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.11
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.11
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.11
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.11
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB2	12	0.11
(2,654)	1:692:A:LEU:HD11	1:691:A:SER:HB3	12	0.11
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB2	12	0.11
(2,654)	1:692:A:LEU:HD12	1:691:A:SER:HB3	12	0.11
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB2	12	0.11
(2,654)	1:692:A:LEU:HD13	1:691:A:SER:HB3	12	0.11
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	6	0.11
(2,649)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	6	0.11
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	6	0.11
(2,649)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	6	0.11
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	6	0.11
(2,649)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	6	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.11
(2,645)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.11
(2,645)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.11
(2,645)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.11
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.11
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.11
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.11
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.11
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.11
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.11
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.11
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.11
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.11
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.11
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.11
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.11
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.11
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.11
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.11
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.11
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.11
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.11
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.11
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.11
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.11
(2,619)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.11
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.11
(2,619)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.11
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.11
(2,619)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.11
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.11
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.11
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.11
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.11
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.11
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.11
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.11
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.11
(2,608)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.11
(2,586)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.11
(2,581)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.11
(2,581)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(2,580)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(2,580)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(2,580)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(2,580)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(2,580)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,580)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(2,564)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.11
(2,556)	1:666:A:TRP:H	1:663:A:LEU:HA	13	0.11
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	0.11
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	0.11
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	0.11
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	0.11
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	0.11
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	0.11
(2,536)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	0.11
(2,534)	1:770:A:ARG:HH22	1:773:A:ASP:OD1	13	0.11
(2,493)	1:781:A:ILE:H	1:778:A:VAL:HA	12	0.11
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD2	2	0.11
(2,476)	1:777:A:ILE:HG21	1:780:A:ARG:HD3	2	0.11
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD2	2	0.11
(2,476)	1:777:A:ILE:HG22	1:780:A:ARG:HD3	2	0.11
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD2	2	0.11
(2,476)	1:777:A:ILE:HG23	1:780:A:ARG:HD3	2	0.11
(2,464)	1:776:A:LEU:H	1:773:A:ASP:HA	3	0.11
(2,458)	1:775:A:LEU:H	1:772:A:ARG:HA	13	0.11
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE1	9	0.11
(2,445)	1:771:A:LEU:HD11	1:768:A:TYR:HE2	9	0.11
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE1	9	0.11
(2,445)	1:771:A:LEU:HD12	1:768:A:TYR:HE2	9	0.11
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE1	9	0.11
(2,445)	1:771:A:LEU:HD13	1:768:A:TYR:HE2	9	0.11
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	13	0.11
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	2	0.11
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	2	0.11
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	2	0.11
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	2	0.11
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	2	0.11
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	2	0.11
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	9	0.11
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	9	0.11
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	9	0.11
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	9	0.11
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	9	0.11
(2,428)	1:758:A:ASP:H	1:754:A:ALA:HB1	7	0.11
(2,428)	1:758:A:ASP:H	1:754:A:ALA:HB2	7	0.11
(2,428)	1:758:A:ASP:H	1:754:A:ALA:HB3	7	0.11
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	8	0.11
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	8	0.11
(2,415)	1:754:A:ALA:HB1	1:758:A:ASP:H	7	0.11
(2,415)	1:754:A:ALA:HB2	1:758:A:ASP:H	7	0.11
(2,415)	1:754:A:ALA:HB3	1:758:A:ASP:H	7	0.11
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	14	0.11
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	14	0.11
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	14	0.11
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	14	0.11
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	14	0.11
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	14	0.11
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	5	0.11
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB2	2	0.11
(2,386)	1:746:A:ILE:HD11	1:743:A:ASP:HB3	2	0.11
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB2	2	0.11
(2,386)	1:746:A:ILE:HD12	1:743:A:ASP:HB3	2	0.11
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB2	2	0.11
(2,386)	1:746:A:ILE:HD13	1:743:A:ASP:HB3	2	0.11
(2,383)	1:746:A:ILE:H	1:747:A:ARG:H	9	0.11
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB2	8	0.11
(2,380)	1:746:A:ILE:H	1:743:A:ASP:HB3	8	0.11
(2,361)	1:710:A:GLN:HE21	1:706:A:ASN:HB2	6	0.11
(2,361)	1:710:A:GLN:HE21	1:706:A:ASN:HB3	6	0.11
(2,361)	1:710:A:GLN:HE22	1:706:A:ASN:HB2	6	0.11
(2,361)	1:710:A:GLN:HE22	1:706:A:ASN:HB3	6	0.11
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	13	0.11
(2,353)	1:709:A:ARG:HE	1:709:A:ARG:H	2	0.11
(2,353)	1:709:A:ARG:HE	1:709:A:ARG:H	11	0.11
(2,338)	1:708:A:VAL:H	1:705:A:VAL:HA	11	0.11
(2,329)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.11
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB2	6	0.11
(2,328)	1:707:A:ARG:H	1:703:A:SER:HB3	6	0.11
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.11
(2,311)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.11
(2,311)	1:705:A:VAL:H	1:702:A:LEU:HA	8	0.11
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	8	0.11
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,310)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	8	0.11
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	8	0.11
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	8	0.11
(2,310)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	8	0.11
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	8	0.11
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	8	0.11
(2,310)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	8	0.11
(2,282)	1:700:A:ALA:HB1	1:697:A:ILE:HA	6	0.11
(2,282)	1:700:A:ALA:HB2	1:697:A:ILE:HA	6	0.11
(2,282)	1:700:A:ALA:HB3	1:697:A:ILE:HA	6	0.11
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.11
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.11
(2,269)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.11
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.11
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.11
(2,269)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.11
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.11
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.11
(2,269)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.11
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.11
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.11
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.11
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.11
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.11
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.11
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB2	12	0.11
(2,248)	1:692:A:LEU:HD11	1:691:A:SER:HB3	12	0.11
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB2	12	0.11
(2,248)	1:692:A:LEU:HD12	1:691:A:SER:HB3	12	0.11
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB2	12	0.11
(2,248)	1:692:A:LEU:HD13	1:691:A:SER:HB3	12	0.11
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	6	0.11
(2,243)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	6	0.11
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	6	0.11
(2,243)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	6	0.11
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,243)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	6	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.11
(2,239)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.11
(2,239)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.11
(2,239)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.11
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.11
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.11
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.11
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.11
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.11
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.11
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.11
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.11
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.11
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.11
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.11
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.11
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	9	0.11
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	9	0.11
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	9	0.11
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.11
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.11
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.11
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.11
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.11
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.11
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.11
(2,213)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.11
(2,213)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.11
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.11
(2,213)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.11
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.11
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.11
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.11
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.11
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.11
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.11
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.11
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.11
(2,202)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.11
(2,180)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.11
(2,175)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.11
(2,175)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(2,174)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(2,174)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(2,174)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(2,174)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(2,174)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11
(2,174)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(2,158)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.11
(2,150)	1:666:A:TRP:H	1:663:A:LEU:HA	13	0.11
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	0.11
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	0.11
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	0.11
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	0.11
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	0.11
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	0.11
(2,130)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	0.11
(2,1345)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	5	0.1
(2,1317)	1:783:A:GLU:H	1:780:A:ARG:HA	13	0.1
(2,1287)	1:777:A:ILE:HD11	1:774:A:LEU:HA	6	0.1
(2,1287)	1:777:A:ILE:HD12	1:774:A:LEU:HA	6	0.1
(2,1287)	1:777:A:ILE:HD13	1:774:A:LEU:HA	6	0.1
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	7	0.1
(2,1281)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	7	0.1
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	7	0.1
(2,1281)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	7	0.1
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	7	0.1
(2,1281)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	7	0.1
(2,1253)	1:764:A:SER:H	1:761:A:ARG:HA	15	0.1
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	6	0.1
(2,1251)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	6	0.1
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	6	0.1
(2,1251)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	6	0.1
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	6	0.1
(2,1251)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	6	0.1
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	4	0.1
(2,1237)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	4	0.1
(2,1236)	1:757:A:TRP:HE1	1:753:A:LEU:HG	5	0.1
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	9	0.1
(2,1218)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	9	0.1
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	9	0.1
(2,1218)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	9	0.1
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	9	0.1
(2,1218)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	9	0.1
(2,1213)	1:753:A:LEU:H	1:750:A:ASN:HB2	7	0.1
(2,1213)	1:753:A:LEU:H	1:750:A:ASN:HB3	7	0.1
(2,1206)	1:748:A:LEU:H	1:745:A:SER:HA	4	0.1
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD2	1	0.1
(2,1205)	1:748:A:LEU:H	1:744:A:ARG:HD3	1	0.1
(2,1202)	1:747:A:ARG:H	1:746:A:ILE:HA	12	0.1
(2,1166)	1:710:A:GLN:H	1:708:A:VAL:HA	2	0.1
(2,1165)	1:709:A:ARG:HE	1:709:A:ARG:H	12	0.1
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.1
(2,1134)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.1
(2,1123)	1:705:A:VAL:H	1:702:A:LEU:HA	15	0.1
(2,1094)	1:700:A:ALA:HB1	1:697:A:ILE:HA	13	0.1
(2,1094)	1:700:A:ALA:HB2	1:697:A:ILE:HA	13	0.1
(2,1094)	1:700:A:ALA:HB3	1:697:A:ILE:HA	13	0.1
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1085)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.1
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.1
(2,1085)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.1
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.1
(2,1085)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.1
(2,1083)	1:698:A:VAL:HG11	1:695:A:LEU:HG	10	0.1
(2,1083)	1:698:A:VAL:HG12	1:695:A:LEU:HG	10	0.1
(2,1083)	1:698:A:VAL:HG13	1:695:A:LEU:HG	10	0.1
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.1
(2,1079)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.1
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.1
(2,1079)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.1
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.1
(2,1079)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.1
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	7	0.1
(2,1072)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	7	0.1
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	7	0.1
(2,1072)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	7	0.1
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	7	0.1
(2,1072)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	7	0.1
(2,1050)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.1
(2,1050)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.1
(2,1050)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.1
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,1033)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,1033)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,1033)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	1	0.1
(2,1030)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	1	0.1
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	1	0.1
(2,1030)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	1	0.1
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	1	0.1
(2,1030)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	1	0.1
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.1
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.1
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.1
(2,1029)	1:684:A:ILE:HD11	1:681:A:TYR:HA	15	0.1
(2,1029)	1:684:A:ILE:HD12	1:681:A:TYR:HA	15	0.1
(2,1029)	1:684:A:ILE:HD13	1:681:A:TYR:HA	15	0.1
(2,1024)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1024)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.1
(2,1024)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.1
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.1
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.1
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.1
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.1
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.1
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.1
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,1023)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,1023)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,1023)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,1004)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.1
(2,1004)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.1
(2,1004)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.1
(2,1000)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.1
(2,939)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	1	0.1
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	5	0.1
(2,911)	1:783:A:GLU:H	1:780:A:ARG:HA	13	0.1
(2,881)	1:777:A:ILE:HD11	1:774:A:LEU:HA	6	0.1
(2,881)	1:777:A:ILE:HD12	1:774:A:LEU:HA	6	0.1
(2,881)	1:777:A:ILE:HD13	1:774:A:LEU:HA	6	0.1
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	7	0.1
(2,875)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	7	0.1
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	7	0.1
(2,875)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	7	0.1
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	7	0.1
(2,875)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	7	0.1
(2,847)	1:764:A:SER:H	1:761:A:ARG:HA	15	0.1
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	6	0.1
(2,845)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	6	0.1
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	6	0.1
(2,845)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	6	0.1
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	6	0.1
(2,845)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	6	0.1
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	4	0.1
(2,831)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	4	0.1
(2,830)	1:757:A:TRP:HE1	1:753:A:LEU:HG	5	0.1
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	9	0.1
(2,812)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	9	0.1
(2,812)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	9	0.1
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	9	0.1
(2,812)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	9	0.1
(2,807)	1:753:A:LEU:H	1:750:A:ASN:HB2	7	0.1
(2,807)	1:753:A:LEU:H	1:750:A:ASN:HB3	7	0.1
(2,800)	1:748:A:LEU:H	1:745:A:SER:HA	4	0.1
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD2	1	0.1
(2,799)	1:748:A:LEU:H	1:744:A:ARG:HD3	1	0.1
(2,796)	1:747:A:ARG:H	1:746:A:ILE:HA	12	0.1
(2,760)	1:710:A:GLN:H	1:708:A:VAL:HA	2	0.1
(2,759)	1:709:A:ARG:HE	1:709:A:ARG:H	12	0.1
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.1
(2,728)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.1
(2,717)	1:705:A:VAL:H	1:702:A:LEU:HA	15	0.1
(2,688)	1:700:A:ALA:HB1	1:697:A:ILE:HA	13	0.1
(2,688)	1:700:A:ALA:HB2	1:697:A:ILE:HA	13	0.1
(2,688)	1:700:A:ALA:HB3	1:697:A:ILE:HA	13	0.1
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.1
(2,679)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.1
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.1
(2,679)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.1
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.1
(2,679)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.1
(2,677)	1:698:A:VAL:HG11	1:695:A:LEU:HG	10	0.1
(2,677)	1:698:A:VAL:HG12	1:695:A:LEU:HG	10	0.1
(2,677)	1:698:A:VAL:HG13	1:695:A:LEU:HG	10	0.1
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.1
(2,673)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.1
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.1
(2,673)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.1
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.1
(2,673)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.1
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	7	0.1
(2,666)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	7	0.1
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	7	0.1
(2,666)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	7	0.1
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	7	0.1
(2,666)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	7	0.1
(2,644)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.1
(2,644)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.1
(2,644)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,627)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,627)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,627)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	1	0.1
(2,624)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	1	0.1
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	1	0.1
(2,624)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	1	0.1
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	1	0.1
(2,624)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	1	0.1
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.1
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.1
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.1
(2,623)	1:684:A:ILE:HD11	1:681:A:TYR:HA	15	0.1
(2,623)	1:684:A:ILE:HD12	1:681:A:TYR:HA	15	0.1
(2,623)	1:684:A:ILE:HD13	1:681:A:TYR:HA	15	0.1
(2,618)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.1
(2,618)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.1
(2,618)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.1
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.1
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.1
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.1
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.1
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.1
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.1
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,617)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,617)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,617)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,598)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.1
(2,598)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.1
(2,598)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.1
(2,594)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.1
(2,533)	1:761:A:ARG:HH21	1:758:A:ASP:OD2	1	0.1
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	5	0.1
(2,505)	1:783:A:GLU:H	1:780:A:ARG:HA	13	0.1
(2,475)	1:777:A:ILE:HD11	1:774:A:LEU:HA	6	0.1
(2,475)	1:777:A:ILE:HD12	1:774:A:LEU:HA	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,475)	1:777:A:ILE:HD13	1:774:A:LEU:HA	6	0.1
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB2	7	0.1
(2,469)	1:776:A:LEU:HD11	1:773:A:ASP:HB3	7	0.1
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB2	7	0.1
(2,469)	1:776:A:LEU:HD12	1:773:A:ASP:HB3	7	0.1
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB2	7	0.1
(2,469)	1:776:A:LEU:HD13	1:773:A:ASP:HB3	7	0.1
(2,441)	1:764:A:SER:H	1:761:A:ARG:HA	15	0.1
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE1	6	0.1
(2,439)	1:763:A:LEU:HD21	1:768:A:TYR:HE2	6	0.1
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE1	6	0.1
(2,439)	1:763:A:LEU:HD22	1:768:A:TYR:HE2	6	0.1
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE1	6	0.1
(2,439)	1:763:A:LEU:HD23	1:768:A:TYR:HE2	6	0.1
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB2	4	0.1
(2,425)	1:757:A:TRP:HE1	1:760:A:LEU:HB3	4	0.1
(2,424)	1:757:A:TRP:HE1	1:753:A:LEU:HG	5	0.1
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB2	9	0.1
(2,406)	1:753:A:LEU:HD11	1:757:A:TRP:HB3	9	0.1
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB2	9	0.1
(2,406)	1:753:A:LEU:HD12	1:757:A:TRP:HB3	9	0.1
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB2	9	0.1
(2,406)	1:753:A:LEU:HD13	1:757:A:TRP:HB3	9	0.1
(2,401)	1:753:A:LEU:H	1:750:A:ASN:HB2	7	0.1
(2,401)	1:753:A:LEU:H	1:750:A:ASN:HB3	7	0.1
(2,394)	1:748:A:LEU:H	1:745:A:SER:HA	4	0.1
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD2	1	0.1
(2,393)	1:748:A:LEU:H	1:744:A:ARG:HD3	1	0.1
(2,390)	1:747:A:ARG:H	1:746:A:ILE:HA	12	0.1
(2,354)	1:710:A:GLN:H	1:708:A:VAL:HA	2	0.1
(2,353)	1:709:A:ARG:HE	1:709:A:ARG:H	12	0.1
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.1
(2,322)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.1
(2,311)	1:705:A:VAL:H	1:702:A:LEU:HA	15	0.1
(2,282)	1:700:A:ALA:HB1	1:697:A:ILE:HA	13	0.1
(2,282)	1:700:A:ALA:HB2	1:697:A:ILE:HA	13	0.1
(2,282)	1:700:A:ALA:HB3	1:697:A:ILE:HA	13	0.1
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.1
(2,273)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.1
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.1
(2,273)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.1
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,273)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.1
(2,271)	1:698:A:VAL:HG11	1:695:A:LEU:HG	10	0.1
(2,271)	1:698:A:VAL:HG12	1:695:A:LEU:HG	10	0.1
(2,271)	1:698:A:VAL:HG13	1:695:A:LEU:HG	10	0.1
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.1
(2,267)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.1
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.1
(2,267)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.1
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.1
(2,267)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.1
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	7	0.1
(2,260)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	7	0.1
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	7	0.1
(2,260)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	7	0.1
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	7	0.1
(2,260)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	7	0.1
(2,238)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.1
(2,238)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.1
(2,238)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.1
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,221)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,221)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,221)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	1	0.1
(2,218)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	1	0.1
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	1	0.1
(2,218)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	1	0.1
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	1	0.1
(2,218)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	1	0.1
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.1
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.1
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.1
(2,217)	1:684:A:ILE:HD11	1:681:A:TYR:HA	15	0.1
(2,217)	1:684:A:ILE:HD12	1:681:A:TYR:HA	15	0.1
(2,217)	1:684:A:ILE:HD13	1:681:A:TYR:HA	15	0.1
(2,212)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.1
(2,212)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.1
(2,212)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.1
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.1
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.1
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.1
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.1
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.1
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.1
(2,211)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.1
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.1
(2,211)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.1
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.1
(2,211)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.1
(2,192)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.1
(2,192)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.1
(2,192)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.1
(2,188)	1:674:A:ASP:H	1:677:A:ASN:H	2	0.1
(1,75)	1:756:C:ILE:O	1:760:C:LEU:H	8	0.1
(1,49)	1:756:C:ILE:O	1:760:C:LEU:H	8	0.1
(1,23)	1:756:C:ILE:O	1:760:C:LEU:H	8	0.1

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

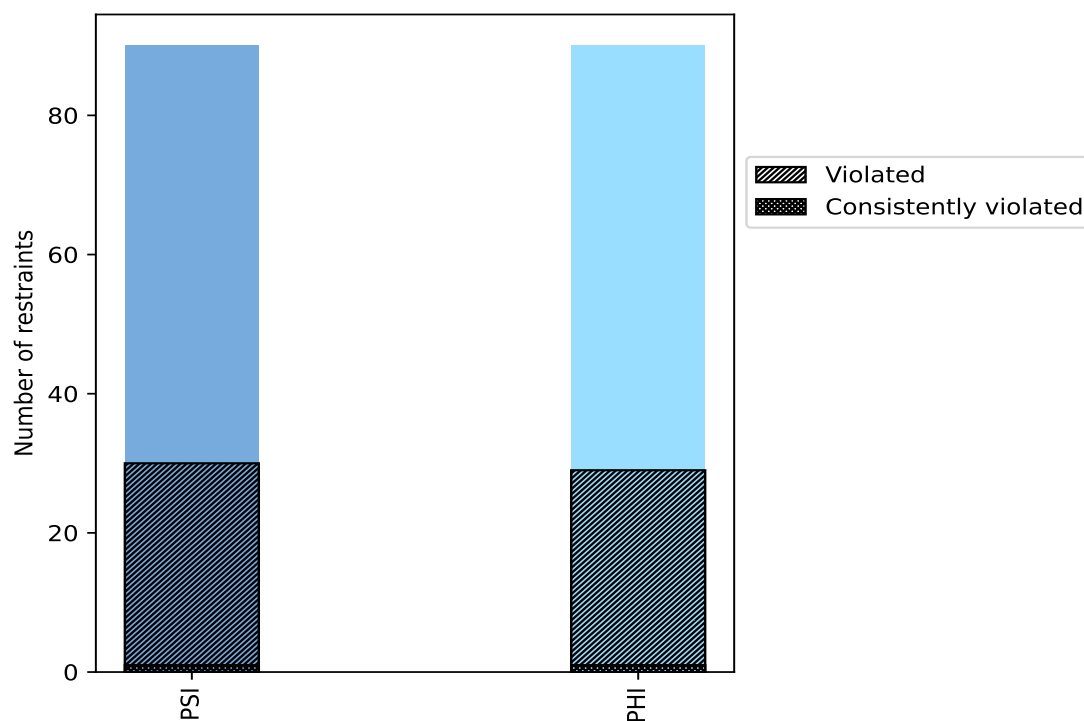
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	90	50.0	30	33.3	16.7	1	1.1	0.6
PHI	90	50.0	29	32.2	16.1	1	1.1	0.6
Total	180	100.0	59	32.8	32.8	2	1.1	1.1

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

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



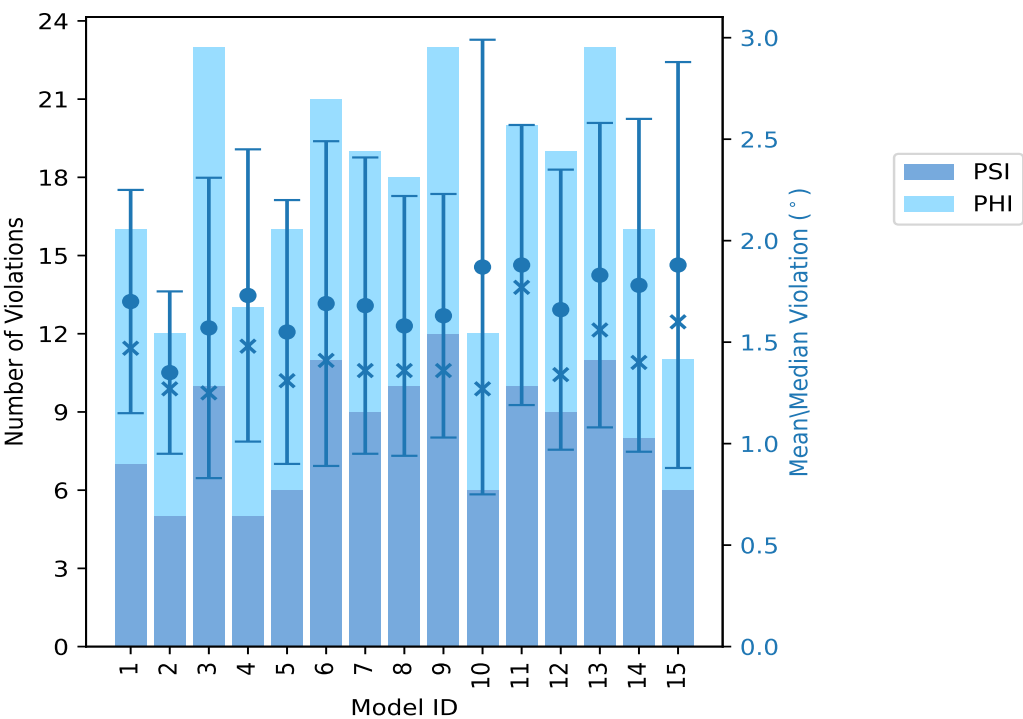
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	7	9	16	1.7	2.83	0.55	1.47
2	5	7	12	1.35	2.53	0.4	1.27
3	10	13	23	1.57	3.6	0.74	1.25
4	5	8	13	1.73	3.29	0.72	1.48
5	6	10	16	1.55	3.41	0.65	1.31
6	11	10	21	1.69	3.83	0.8	1.41
7	9	10	19	1.68	3.67	0.73	1.36
8	10	8	18	1.58	3.32	0.64	1.36
9	12	11	23	1.63	3.02	0.6	1.36
10	6	6	12	1.87	4.34	1.12	1.27
11	10	10	20	1.88	3.44	0.69	1.77
12	9	10	19	1.66	3.31	0.69	1.34
13	11	12	23	1.83	3.64	0.75	1.56
14	8	8	16	1.78	3.7	0.82	1.4
15	6	5	11	1.88	3.94	1.0	1.6

10.2.1 Bar graph : Dihedral 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

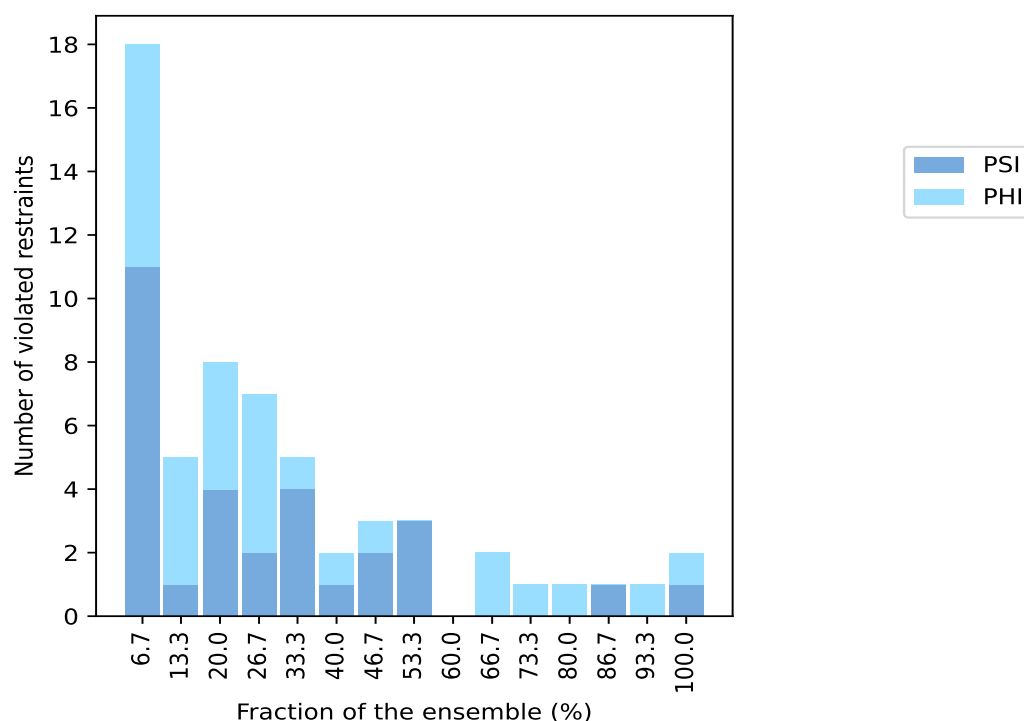
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
11	7	18	1	6.7
1	4	5	2	13.3
4	4	8	3	20.0
2	5	7	4	26.7
4	1	5	5	33.3
1	1	2	6	40.0
2	1	3	7	46.7
3	0	3	8	53.3
0	0	0	9	60.0
0	2	2	10	66.7
0	1	1	11	73.3
0	1	1	12	80.0
1	0	1	13	86.7
0	1	1	14	93.3
1	1	2	15	100.0

¹ Number of models with violations

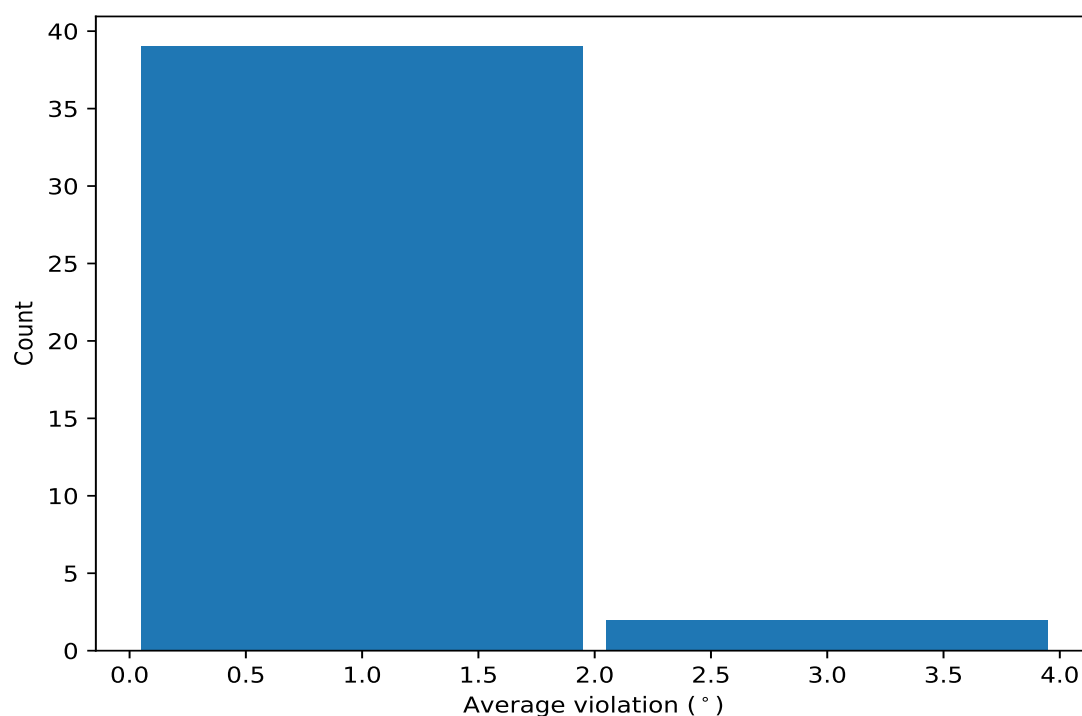
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	15	3.37	0.6	3.43
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	15	3.21	0.73	3.24
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	14	1.74	0.36	1.62
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	13	1.45	0.37	1.47
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	12	1.84	0.61	1.65
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	11	1.63	0.34	1.57
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	10	1.95	0.34	1.91
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	10	1.27	0.18	1.28
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	8	1.65	0.42	1.68
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	8	1.5	0.13	1.54
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	8	1.35	0.36	1.23
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	7	1.75	0.56	1.52
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	7	1.71	0.5	1.54
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	7	1.31	0.23	1.23
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	6	1.8	0.39	1.86
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	6	1.26	0.12	1.27
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	5	1.78	0.52	1.74
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	5	1.48	0.71	1.13
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	5	1.33	0.17	1.37
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	5	1.33	0.18	1.36
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	5	1.17	0.14	1.15

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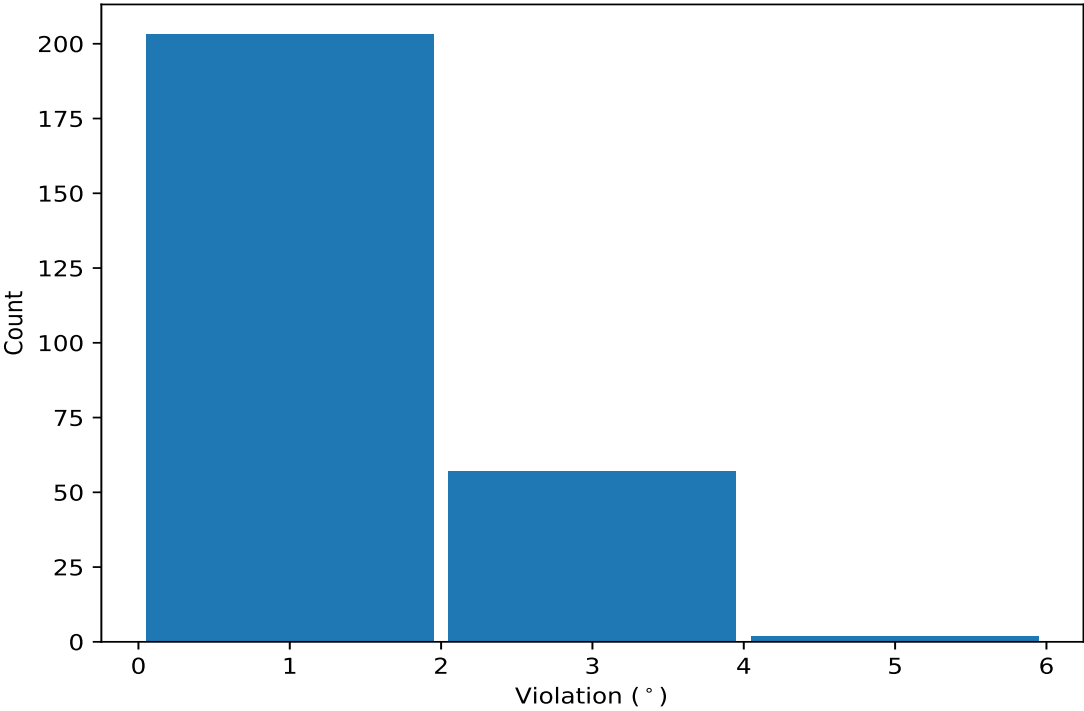
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,82)	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	1:710:C:GLN:N	4	1.44	0.22	1.42
(1,61)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	4	1.33	0.45	1.1
(1,157)	1:774:C:LEU:C	1:775:C:LEU:N	1:775:C:LEU:CA	1:775:C:LEU:C	4	1.29	0.19	1.31
(1,165)	1:778:C:VAL:C	1:779:C:THR:N	1:779:C:THR:CA	1:779:C:THR:C	4	1.26	0.11	1.25
(1,75)	1:705:C:VAL:C	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	4	1.16	0.13	1.1
(1,176)	1:784:C:LEU:N	1:784:C:LEU:CA	1:784:C:LEU:C	1:785:C:LEU:N	4	1.13	0.15	1.06
(1,59)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	4	1.11	0.1	1.07
(1,62)	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	1:700:C:ALA:N	3	1.67	0.74	1.29
(1,63)	1:699:C:PHE:C	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	3	1.51	0.31	1.42
(1,80)	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	1:709:C:ARG:N	3	1.51	0.39	1.56
(1,156)	1:774:C:LEU:N	1:774:C:LEU:CA	1:774:C:LEU:C	1:775:C:LEU:N	3	1.34	0.18	1.4
(1,127)	1:754:C:ALA:C	1:755:C:LEU:N	1:755:C:LEU:CA	1:755:C:LEU:C	3	1.32	0.09	1.29
(1,46)	1:691:C:SER:N	1:691:C:SER:CA	1:691:C:SER:C	1:692:C:LEU:N	3	1.18	0.09	1.2
(1,119)	1:750:C:ASN:C	1:751:C:GLY:N	1:751:C:GLY:CA	1:751:C:GLY:C	3	1.18	0.11	1.14
(1,159)	1:775:C:LEU:C	1:776:C:LEU:N	1:776:C:LEU:CA	1:776:C:LEU:C	3	1.11	0.02	1.12
(1,81)	1:708:C:VAL:C	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	2	1.42	0.1	1.42
(1,18)	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	1:676:C:THR:N	2	1.28	0.05	1.28
(1,163)	1:777:C:ILE:C	1:778:C:VAL:N	1:778:C:VAL:CA	1:778:C:VAL:C	2	1.27	0.03	1.27
(1,103)	1:742:C:ARG:C	1:743:C:ASP:N	1:743:C:ASP:CA	1:743:C:ASP:C	2	1.24	0.21	1.24
(1,177)	1:784:C:LEU:C	1:785:C:LEU:N	1:785:C:LEU:CA	1:785:C:LEU:C	2	1.14	0.06	1.14

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	10	4.34
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	10	4.15
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	15	3.94
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	15	3.87
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	6	3.83
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	6	3.72
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	14	3.7
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	7	3.67
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	13	3.64
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	13	3.63
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	3	3.6
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	3.56
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	11	3.44
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	11	3.43
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	5	3.41
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	3	3.39
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	8	3.32
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	12	3.31
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	4	3.29
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	8	3.24
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	12	3.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	4	3.21
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	7	3.21
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	6	3.1
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	9	3.02
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	13	2.92
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	13	2.9
(1,168)	1:780:C:ARG:N	1:780:C:ARG:CA	1:780:C:ARG:C	1:781:C:ILE:N	14	2.87
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	1	2.83
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	9	2.82
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	3	2.79
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1	2.74
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	5	2.73
(1,62)	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	1:700:C:ALA:N	11	2.7
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	9	2.69
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	9	2.64
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	7	2.58
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	2	2.53
(1,88)	1:715:C:LEU:N	1:715:C:LEU:CA	1:715:C:LEU:C	1:716:C:SER:N	1	2.5
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	11	2.32
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	11	2.3
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	10	2.29
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	3	2.28
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	12	2.28
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	13	2.27
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	7	2.26
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	12	2.25
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	4	2.21
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	11	2.21
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	9	2.19
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1	2.13
(1,61)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	11	2.1
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	13	2.08
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	12	2.06
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1	2.04
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	3	2.03
(1,169)	1:780:C:ARG:C	1:781:C:ILE:N	1:781:C:ILE:CA	1:781:C:ILE:C	14	2.02
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	5	2.0
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	7	2.0
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	13	1.99
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	6	1.98
(1,80)	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	1:709:C:ARG:N	11	1.96
(1,63)	1:699:C:PHE:C	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	11	1.93
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	9	1.92
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	12	1.9
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	15	1.9
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	8	1.9
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	10	1.89
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	13	1.87
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	14	1.86
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	5	1.85
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	12	1.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	9	1.82
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	4	1.8
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	15	1.8
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	13	1.78
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	11	1.77
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	11	1.77
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	8	1.74
(1,82)	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	1:710:C:GLN:N	13	1.73
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	9	1.72
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	4	1.69
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	15	1.67
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	13	1.67
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	8	1.66
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	12	1.66
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	7	1.66
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	7	1.65
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	12	1.64
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	3	1.63
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	1	1.6
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	15	1.6
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	14	1.59
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	10	1.59
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	6	1.59
(1,82)	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	1:710:C:GLN:N	6	1.58
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	11	1.58
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	6	1.57
(1,20)	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	1:677:C:ASN:N	6	1.57
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	13	1.56
(1,80)	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	1:709:C:ARG:N	3	1.56
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	4	1.56
(1,160)	1:776:C:LEU:N	1:776:C:LEU:CA	1:776:C:LEU:C	1:777:C:ILE:N	8	1.55
(1,157)	1:774:C:LEU:C	1:775:C:LEU:N	1:775:C:LEU:CA	1:775:C:LEU:C	5	1.55
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	13	1.54
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	6	1.54
(1,156)	1:774:C:LEU:N	1:774:C:LEU:CA	1:774:C:LEU:C	1:775:C:LEU:N	6	1.53
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	1	1.53
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	2	1.53
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	8	1.52
(1,81)	1:708:C:VAL:C	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	11	1.52
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	13	1.51
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	15	1.49
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	3	1.49
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	4	1.48
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	1	1.47
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	5	1.47
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	1	1.47
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	14	1.47
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	7	1.46
(1,56)	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	1:697:C:ILE:N	2	1.46
(1,103)	1:742:C:ARG:C	1:743:C:ASP:N	1:743:C:ASP:CA	1:743:C:ASP:C	5	1.45
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	7	1.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:754:C:ALA:C	1:755:C:LEU:N	1:755:C:LEU:CA	1:755:C:LEU:C	1	1.44
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	11	1.43
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	3	1.43
(1,165)	1:778:C:VAL:C	1:779:C:THR:N	1:779:C:THR:CA	1:779:C:THR:C	1	1.42
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	13	1.42
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	14	1.42
(1,63)	1:699:C:PHE:C	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	2	1.42
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.41
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	11	1.41
(1,156)	1:774:C:LEU:N	1:774:C:LEU:CA	1:774:C:LEU:C	1:775:C:LEU:N	9	1.4
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	1	1.4
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	2	1.4
(1,176)	1:784:C:LEU:N	1:784:C:LEU:CA	1:784:C:LEU:C	1:785:C:LEU:N	14	1.39
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	8	1.39
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	14	1.38
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	5	1.38
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	8	1.38
(1,75)	1:705:C:VAL:C	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	13	1.37
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	9	1.37
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	13	1.37
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	7	1.36
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	9	1.36
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	9	1.36
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	9	1.35
(1,150)	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	1:772:C:ARG:N	11	1.34
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	12	1.34
(1,119)	1:750:C:ASN:C	1:751:C:GLY:N	1:751:C:GLY:CA	1:751:C:GLY:C	7	1.34
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	3	1.34
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	8	1.33
(1,18)	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	1:676:C:THR:N	8	1.33
(1,157)	1:774:C:LEU:C	1:775:C:LEU:N	1:775:C:LEU:CA	1:775:C:LEU:C	9	1.32
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	6	1.32
(1,81)	1:708:C:VAL:C	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	7	1.31
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	10	1.31
(1,171)	1:781:C:ILE:C	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	9	1.3
(1,163)	1:777:C:ILE:C	1:778:C:VAL:N	1:778:C:VAL:CA	1:778:C:VAL:C	13	1.3
(1,117)	1:749:C:VAL:C	1:750:C:ASN:N	1:750:C:ASN:CA	1:750:C:ASN:C	3	1.3
(1,157)	1:774:C:LEU:C	1:775:C:LEU:N	1:775:C:LEU:CA	1:775:C:LEU:C	6	1.29
(1,127)	1:754:C:ALA:C	1:755:C:LEU:N	1:755:C:LEU:CA	1:755:C:LEU:C	9	1.29
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	2	1.29
(1,62)	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	1:700:C:ALA:N	4	1.29
(1,165)	1:778:C:VAL:C	1:779:C:THR:N	1:779:C:THR:CA	1:779:C:THR:C	14	1.28
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	8	1.28
(1,59)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	7	1.28
(1,58)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	13	1.28
(1,46)	1:691:C:SER:N	1:691:C:SER:CA	1:691:C:SER:C	1:692:C:LEU:N	14	1.28
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	14	1.25
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	7	1.25
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	11	1.25
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	6	1.25
(1,82)	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	1:710:C:GLN:N	1	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	3	1.25
(1,163)	1:777:C:ILE:C	1:778:C:VAL:N	1:778:C:VAL:CA	1:778:C:VAL:C	2	1.24
(1,143)	1:762:C:SER:C	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	5	1.24
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	4	1.24
(1,18)	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	1:676:C:THR:N	6	1.24
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	10	1.23
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	15	1.23
(1,167)	1:779:C:THR:C	1:780:C:ARG:N	1:780:C:ARG:CA	1:780:C:ARG:C	4	1.23
(1,149)	1:770:C:ARG:C	1:771:C:LEU:N	1:771:C:LEU:CA	1:771:C:LEU:C	3	1.23
(1,145)	1:763:C:LEU:C	1:764:C:SER:N	1:764:C:SER:CA	1:764:C:SER:C	6	1.23
(1,127)	1:754:C:ALA:C	1:755:C:LEU:N	1:755:C:LEU:CA	1:755:C:LEU:C	13	1.23
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	10	1.23
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	12	1.23
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	6	1.22
(1,165)	1:778:C:VAL:C	1:779:C:THR:N	1:779:C:THR:CA	1:779:C:THR:C	8	1.21
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	8	1.21
(1,21)	1:676:C:THR:C	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	6	1.21
(1,177)	1:784:C:LEU:C	1:785:C:LEU:N	1:785:C:LEU:CA	1:785:C:LEU:C	14	1.2
(1,46)	1:691:C:SER:N	1:691:C:SER:CA	1:691:C:SER:C	1:692:C:LEU:N	9	1.2
(1,82)	1:709:C:ARG:N	1:709:C:ARG:CA	1:709:C:ARG:C	1:710:C:GLN:N	12	1.19
(1,79)	1:707:C:ARG:C	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	5	1.19
(1,63)	1:699:C:PHE:C	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	4	1.19
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	4	1.19
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	9	1.18
(1,83)	1:709:C:ARG:C	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	8	1.17
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.17
(1,40)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	9	1.17
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	3	1.16
(1,144)	1:763:C:LEU:N	1:763:C:LEU:CA	1:763:C:LEU:C	1:764:C:SER:N	9	1.15
(1,75)	1:705:C:VAL:C	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	5	1.15
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	1	1.15
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	2	1.14
(1,119)	1:750:C:ASN:C	1:751:C:GLY:N	1:751:C:GLY:CA	1:751:C:GLY:C	12	1.14
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	10	1.14
(1,159)	1:775:C:LEU:C	1:776:C:LEU:N	1:776:C:LEU:CA	1:776:C:LEU:C	1	1.13
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	10	1.13
(1,159)	1:775:C:LEU:C	1:776:C:LEU:N	1:776:C:LEU:CA	1:776:C:LEU:C	3	1.12
(1,155)	1:773:C:ASP:C	1:774:C:LEU:N	1:774:C:LEU:CA	1:774:C:LEU:C	12	1.12
(1,135)	1:758:C:ASP:C	1:759:C:ASP:N	1:759:C:ASP:CA	1:759:C:ASP:C	2	1.12
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	15	1.12
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	3	1.11
(1,165)	1:778:C:VAL:C	1:779:C:THR:N	1:779:C:THR:CA	1:779:C:THR:C	5	1.11
(1,76)	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	1:707:C:ARG:N	14	1.11
(1,59)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	12	1.11
(1,176)	1:784:C:LEU:N	1:784:C:LEU:CA	1:784:C:LEU:C	1:785:C:LEU:N	9	1.1
(1,154)	1:773:C:ASP:N	1:773:C:ASP:CA	1:773:C:ASP:C	1:774:C:LEU:N	7	1.1
(1,148)	1:770:C:ARG:N	1:770:C:ARG:CA	1:770:C:ARG:C	1:771:C:LEU:N	7	1.1
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	3	1.1
(1,61)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	9	1.1
(1,24)	1:678:C:TRP:N	1:678:C:TRP:CA	1:678:C:TRP:C	1:679:C:LEU:N	7	1.1
(1,159)	1:775:C:LEU:C	1:776:C:LEU:N	1:776:C:LEU:CA	1:776:C:LEU:C	10	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,156)	1:774:C:LEU:N	1:774:C:LEU:CA	1:774:C:LEU:C	1:775:C:LEU:N	5	1.09
(1,126)	1:754:C:ALA:N	1:754:C:ALA:CA	1:754:C:ALA:C	1:755:C:LEU:N	12	1.09
(1,61)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	12	1.09
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	8	1.09
(1,177)	1:784:C:LEU:C	1:785:C:LEU:N	1:785:C:LEU:CA	1:785:C:LEU:C	3	1.08
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	14	1.08
(1,119)	1:750:C:ASN:C	1:751:C:GLY:N	1:751:C:GLY:CA	1:751:C:GLY:C	1	1.07
(1,54)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	5	1.07
(1,46)	1:691:C:SER:N	1:691:C:SER:CA	1:691:C:SER:C	1:692:C:LEU:N	8	1.07
(1,19)	1:675:C:ILE:C	1:676:C:THR:N	1:676:C:THR:CA	1:676:C:THR:C	3	1.07
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	7	1.06
(1,75)	1:705:C:VAL:C	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	10	1.06
(1,60)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	3	1.06
(1,172)	1:782:C:VAL:N	1:782:C:VAL:CA	1:782:C:VAL:C	1:783:C:GLU:N	12	1.05
(1,84)	1:710:C:GLN:N	1:710:C:GLN:CA	1:710:C:GLN:C	1:711:C:GLY:N	12	1.05
(1,75)	1:705:C:VAL:C	1:706:C:ASN:N	1:706:C:ASN:CA	1:706:C:ASN:C	11	1.05
(1,68)	1:702:C:LEU:N	1:702:C:LEU:CA	1:702:C:LEU:C	1:703:C:SER:N	4	1.05
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	15	1.05
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	5	1.05
(1,78)	1:707:C:ARG:N	1:707:C:ARG:CA	1:707:C:ARG:C	1:708:C:VAL:N	13	1.04
(1,176)	1:784:C:LEU:N	1:784:C:LEU:CA	1:784:C:LEU:C	1:785:C:LEU:N	13	1.03
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	2	1.03
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	5	1.03
(1,116)	1:749:C:VAL:N	1:749:C:VAL:CA	1:749:C:VAL:C	1:750:C:ASN:N	6	1.03
(1,103)	1:742:C:ARG:C	1:743:C:ASP:N	1:743:C:ASP:CA	1:743:C:ASP:C	13	1.03
(1,59)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	3	1.03
(1,59)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	11	1.03
(1,22)	1:677:C:ASN:N	1:677:C:ASN:CA	1:677:C:ASN:C	1:678:C:TRP:N	15	1.03
(1,80)	1:708:C:VAL:N	1:708:C:VAL:CA	1:708:C:VAL:C	1:709:C:ARG:N	8	1.02
(1,57)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	2	1.02
(1,55)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	11	1.02
(1,41)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	9	1.02
(1,176)	1:784:C:LEU:N	1:784:C:LEU:CA	1:784:C:LEU:C	1:785:C:LEU:N	6	1.01
(1,157)	1:774:C:LEU:C	1:775:C:LEU:N	1:775:C:LEU:CA	1:775:C:LEU:C	3	1.01
(1,62)	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	1:700:C:ALA:N	2	1.01
(1,61)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	3	1.01
(1,120)	1:751:C:GLY:N	1:751:C:GLY:CA	1:751:C:GLY:C	1:752:C:SER:N	7	1.0