



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 2KNC / pdb_00002knc
BMRB ID : 16496
Title : Platelet integrin ALFAIIB-BETA3 transmembrane-cytoplasmic heterocomplex
Authors : Yang, J.; Ma, Y.; Page, R.C.; Misra, S.; Plow, E.F.; Qin, J.
Deposited on : 2009-08-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

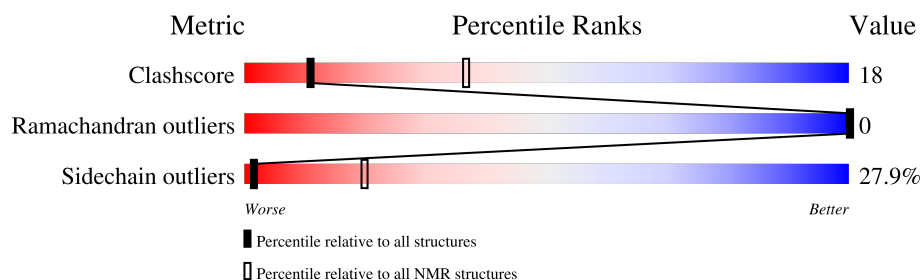
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	54	
2	B	79	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:970-A:988, B:700-B:720 (40)	0.34	5

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2128 atoms, of which 1083 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						Trace
1	A	54	Total	C	H	N	O	S	0
			862	280	435	69	76	2	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	955	GLY	-	expression tag	UNP P08514
A	956	ALA	-	expression tag	UNP P08514
A	957	MET	-	expression tag	UNP P08514
A	958	GLY	-	expression tag	UNP P08514
A	959	SER	-	expression tag	UNP P08514

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						Trace
2	B	79	Total	C	H	N	O	S	0
			1266	401	648	104	111	2	

There are 5 discrepancies between the modelled and reference sequences:

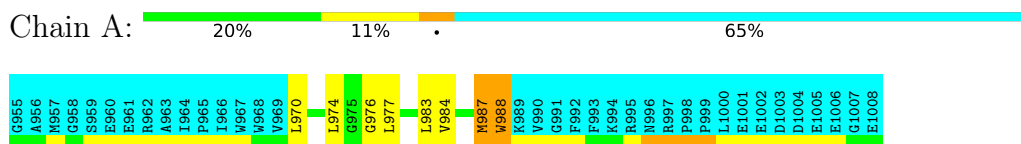
Chain	Residue	Modelled	Actual	Comment	Reference
B	684	GLY	-	expression tag	UNP P05106
B	685	ALA	-	expression tag	UNP P05106
B	686	MET	-	expression tag	UNP P05106
B	687	GLY	-	expression tag	UNP P05106
B	688	SER	-	expression tag	UNP P05106

4 Residue-property plots [i](#)

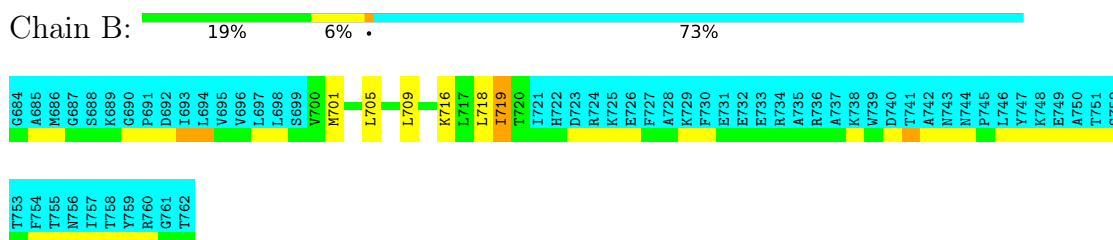
4.1 Average score per residue in the NMR ensemble

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: Integrin alpha-IIb



- Molecule 2: Integrin beta-3

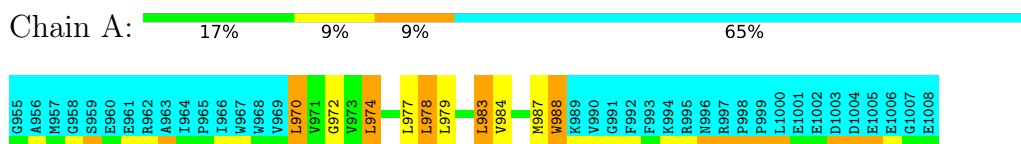


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

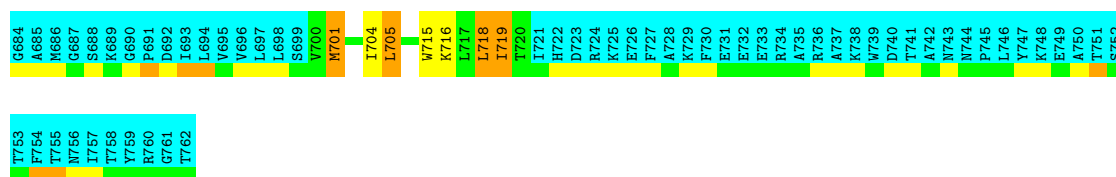
4.2.1 Score per residue for model 1

- Molecule 1: Integrin alpha-IIb



- Molecule 2: Integrin beta-3





4.2.2 Score per residue for model 2

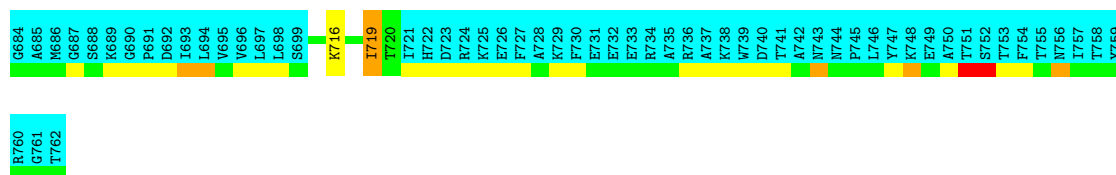
- Molecule 1: Integrin alpha-IIb

Chain A: 20% 9% 6% 65%



- Molecule 2: Integrin beta-3

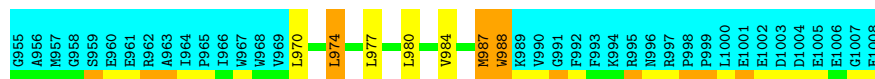
Chain B: 24% .. 73%



4.2.3 Score per residue for model 3

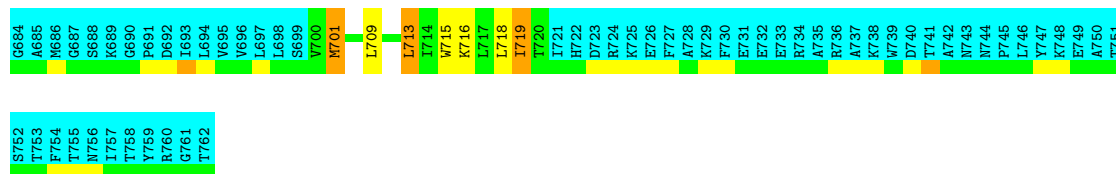
- Molecule 1: Integrin alpha-IIb

Chain A: 22% 7% 6% 65%



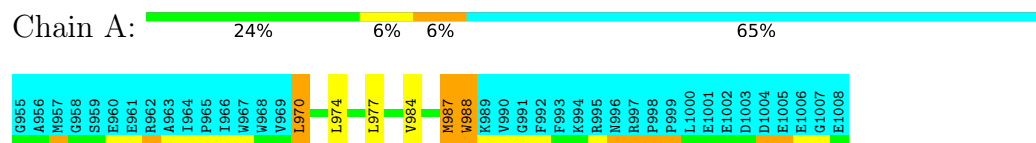
- Molecule 2: Integrin beta-3

Chain B: 18% 5% . 73%

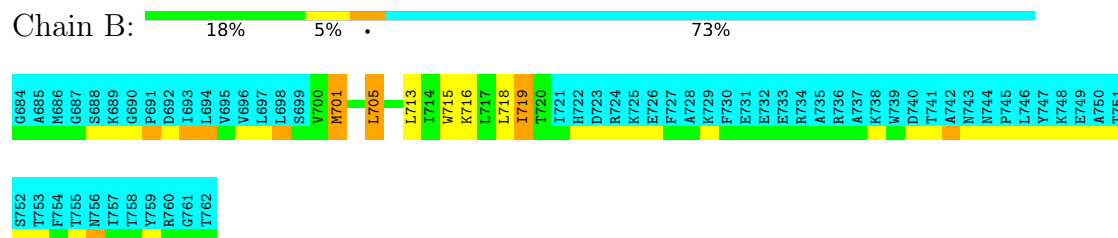


4.2.4 Score per residue for model 4

- Molecule 1: Integrin alpha-IIb

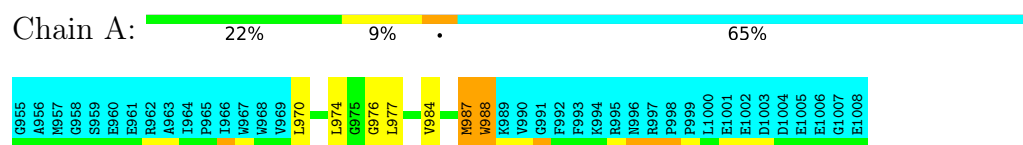


- Molecule 2: Integrin beta-3

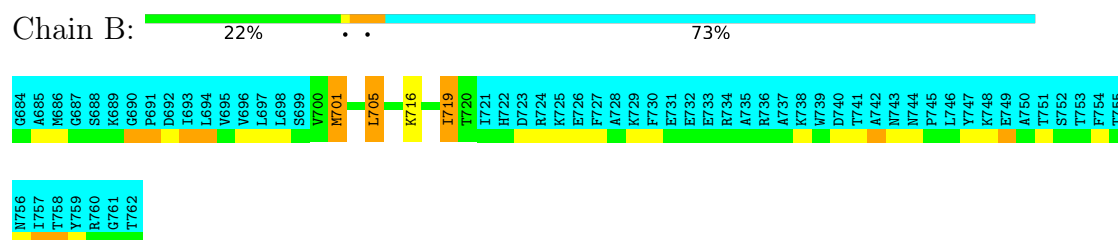


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Integrin alpha-IIb

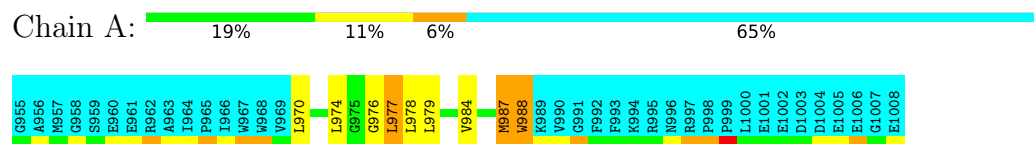


- Molecule 2: Integrin beta-3

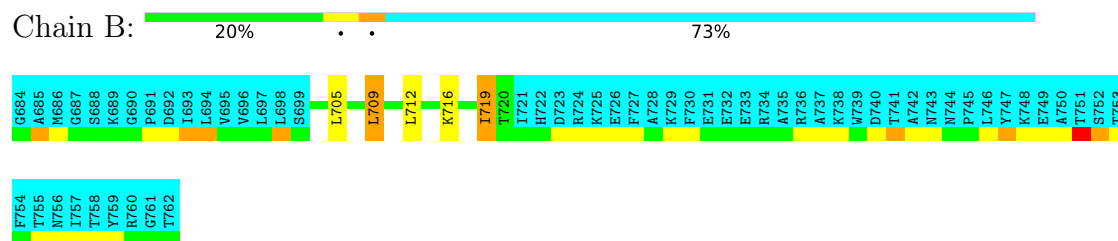


4.2.6 Score per residue for model 6

- Molecule 1: Integrin alpha-IIb

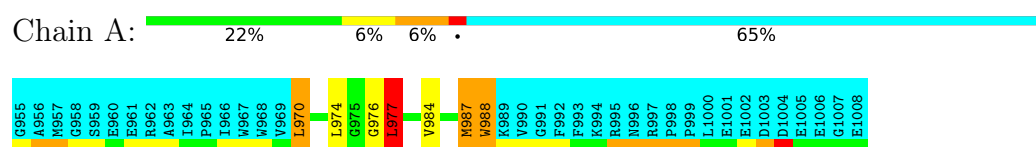


- Molecule 2: Integrin beta-3

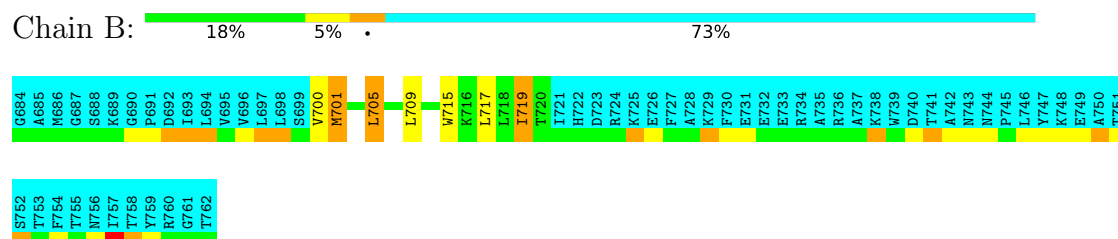


4.2.7 Score per residue for model 7

- Molecule 1: Integrin alpha-IIb

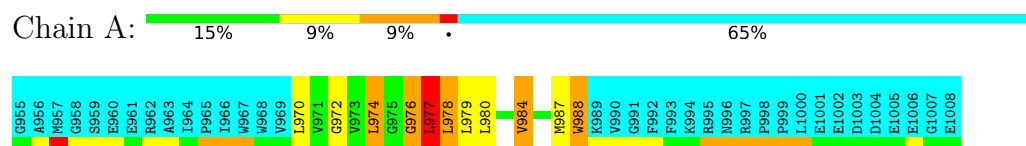


- Molecule 2: Integrin beta-3

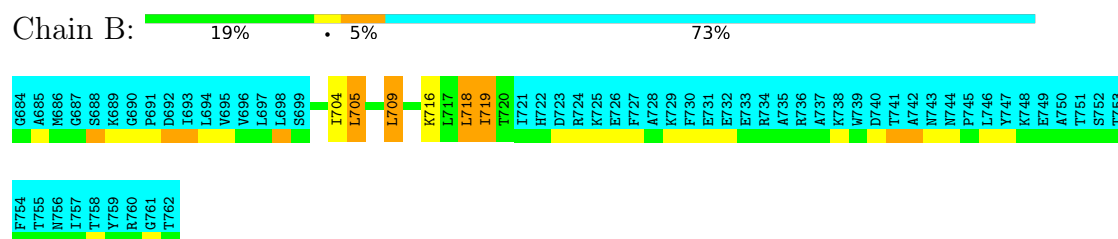


4.2.8 Score per residue for model 8

- Molecule 1: Integrin alpha-IIb

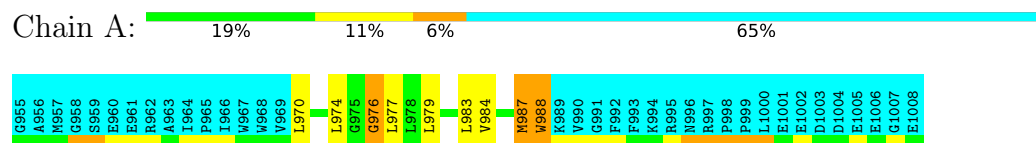


- Molecule 2: Integrin beta-3

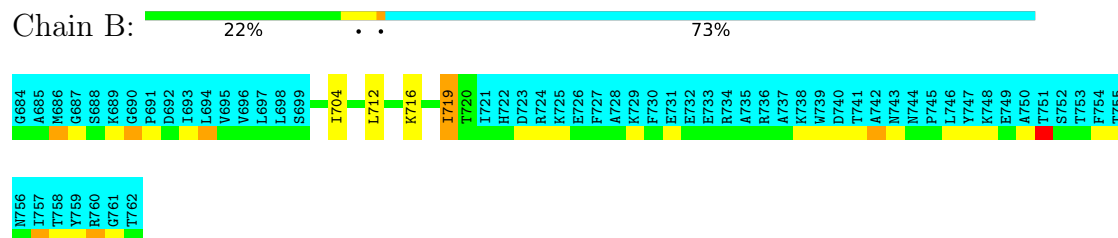


4.2.9 Score per residue for model 9

- Molecule 1: Integrin alpha-IIb

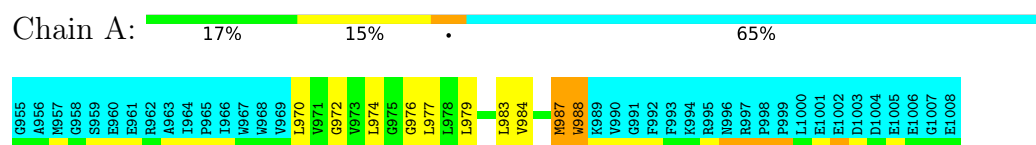


- Molecule 2: Integrin beta-3

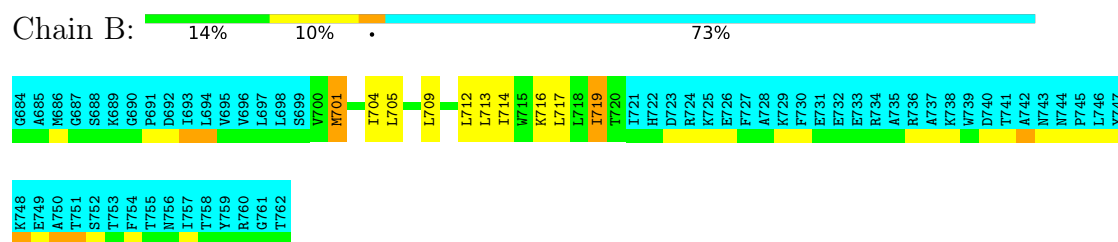


4.2.10 Score per residue for model 10

- Molecule 1: Integrin alpha-IIb

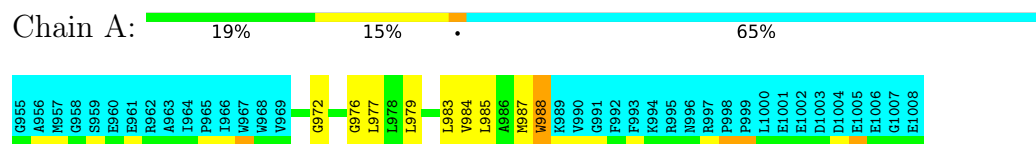


- Molecule 2: Integrin beta-3

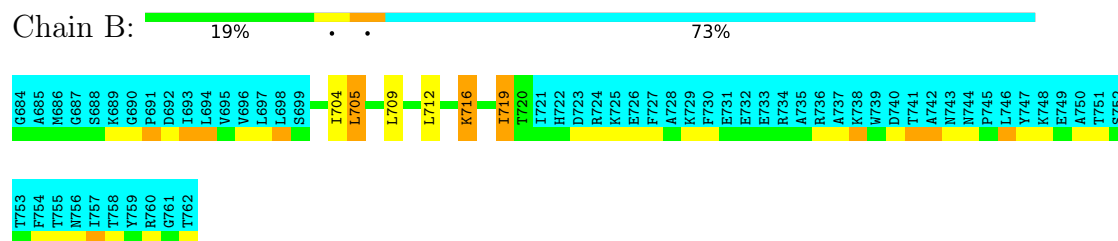


4.2.11 Score per residue for model 11

- Molecule 1: Integrin alpha-IIb

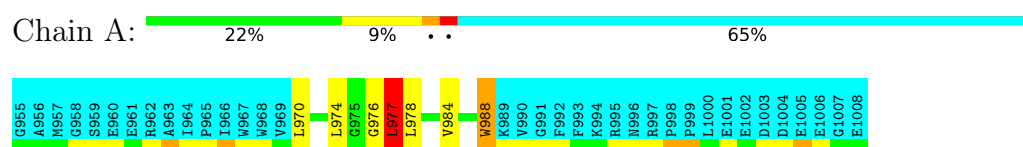


- Molecule 2: Integrin beta-3

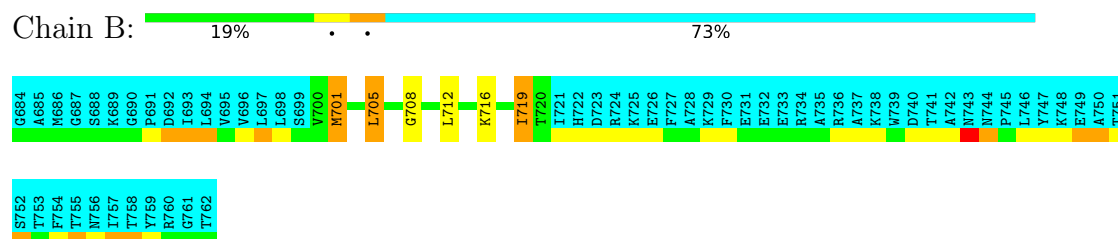


4.2.12 Score per residue for model 12

- Molecule 1: Integrin alpha-IIb

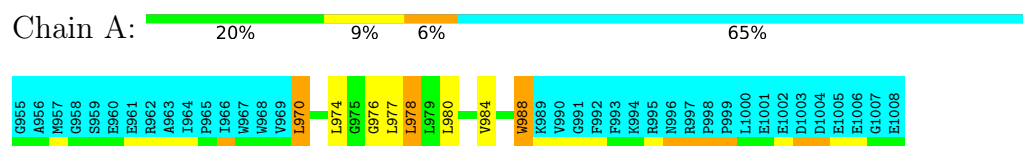


- Molecule 2: Integrin beta-3

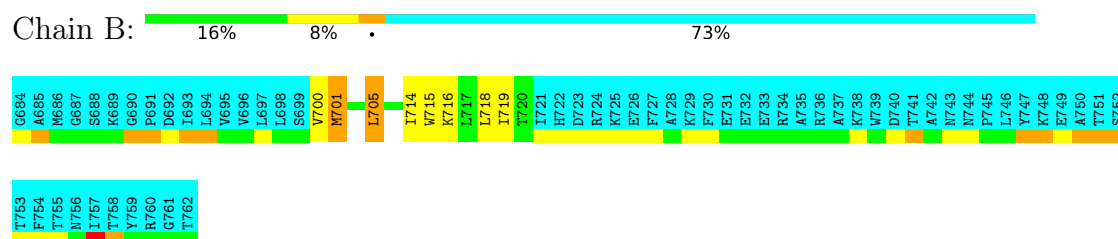


4.2.13 Score per residue for model 13

- Molecule 1: Integrin alpha-IIb

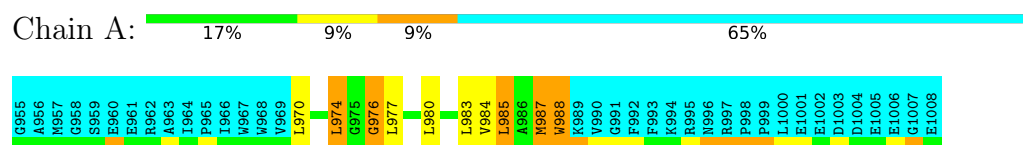


- Molecule 2: Integrin beta-3

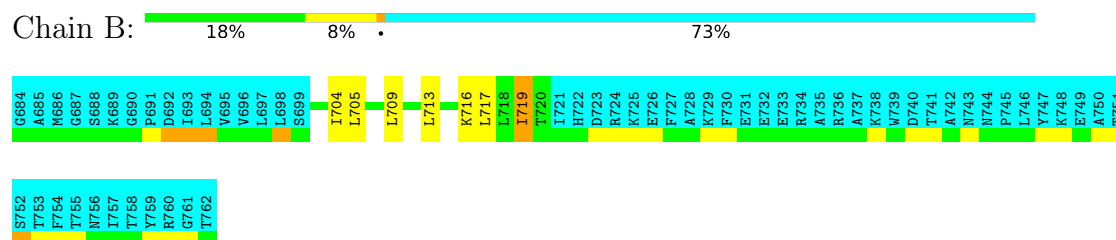


4.2.14 Score per residue for model 14

• Molecule 1: Integrin alpha-IIb

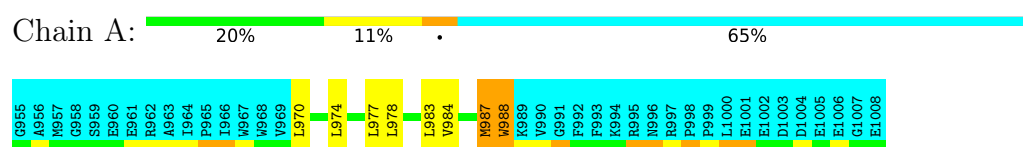


• Molecule 2: Integrin beta-3

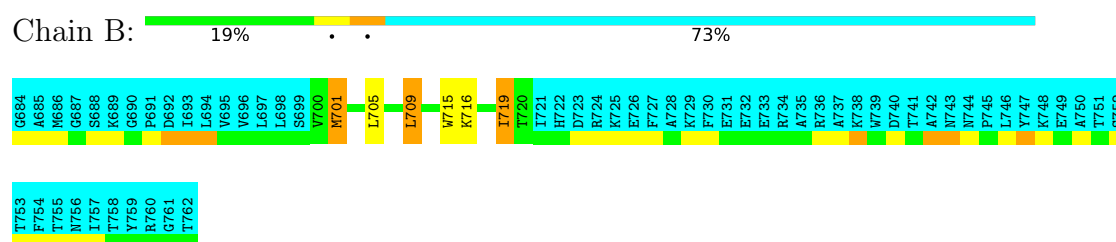


4.2.15 Score per residue for model 15

• Molecule 1: Integrin alpha-IIb

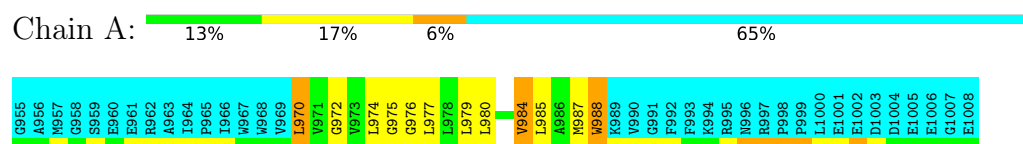


• Molecule 2: Integrin beta-3

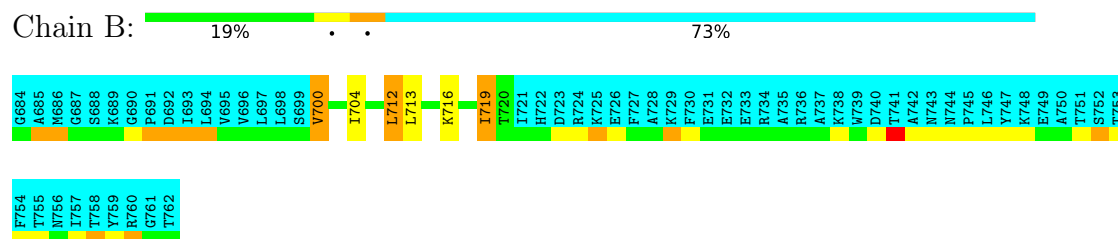


4.2.16 Score per residue for model 16

• Molecule 1: Integrin alpha-IIb

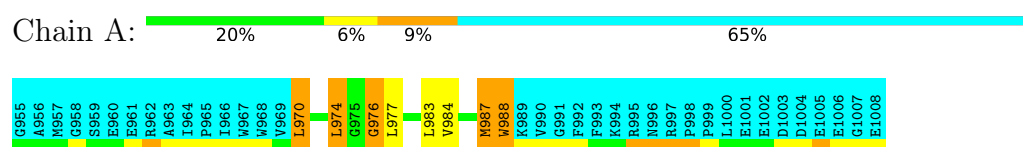


- Molecule 2: Integrin beta-3

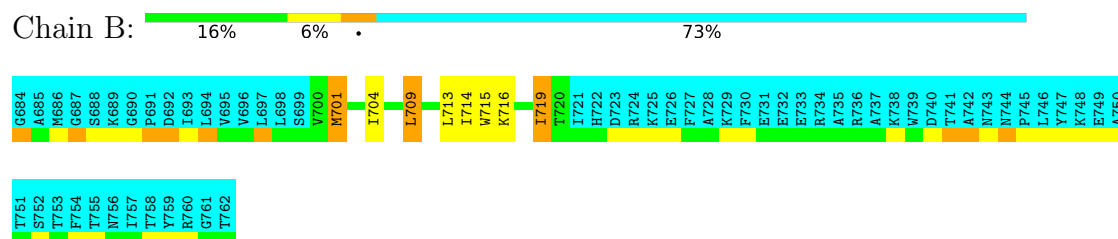


4.2.17 Score per residue for model 17

- Molecule 1: Integrin alpha-IIb

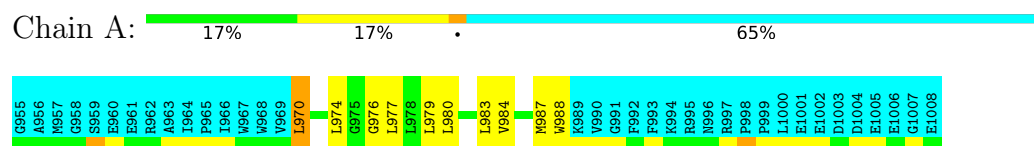


- Molecule 2: Integrin beta-3

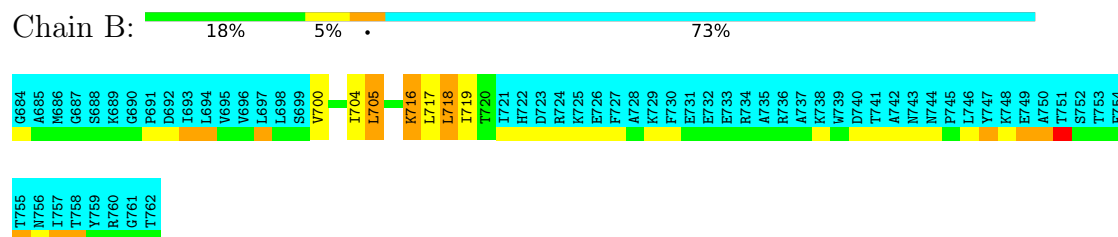


4.2.18 Score per residue for model 18

- Molecule 1: Integrin alpha-IIb



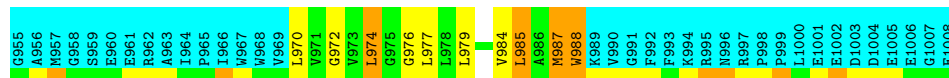
- Molecule 2: Integrin beta-3



4.2.19 Score per residue for model 19

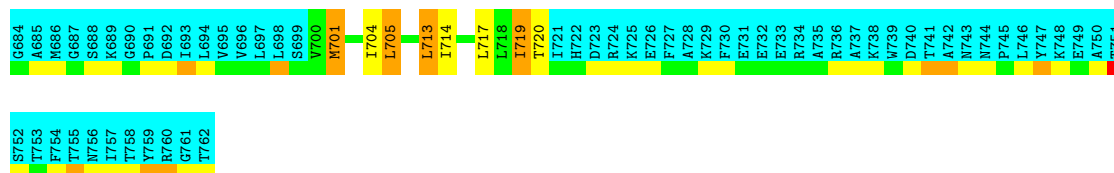
• Molecule 1: Integrin alpha-IIb

Chain A: 



• Molecule 2: Integrin beta-3

Chain B: 



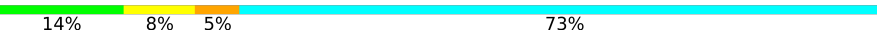
4.2.20 Score per residue for model 20

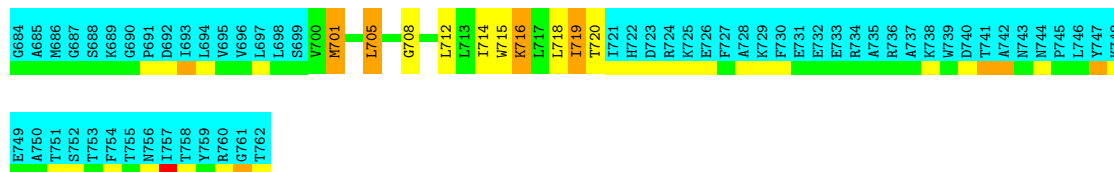
• Molecule 1: Integrin alpha-IIb

Chain A: 



• Molecule 2: Integrin beta-3

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 98 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.15.0
X-PLOR NIH	structure solution	2.15.0

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	1528
Number of shifts mapped to atoms	1528
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	1.54±0.02	0±0/141 (0.0± 0.0%)	1.34±0.02	2±0/194 (0.9± 0.2%)
2	B	1.52±0.02	0±0/158 (0.0± 0.0%)	1.06±0.02	0±0/216 (0.0± 0.0%)
All	All	1.53	0/5980 (0.0%)	1.20	33/8200 (0.4%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	976	GLY	N-CA-C	-6.65	106.12	114.16	7	13
1	A	977	LEU	N-CA-C	-6.25	104.55	111.36	1	20

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	139	166	166	9±3
2	B	156	190	190	7±3
All	All	5900	7120	7120	240

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:987:MET:SD	2:B:719:ILE:HD11	0.81	2.15	3	1
1:A:988:TRP:NE1	2:B:719:ILE:HD11	0.76	1.95	12	8
1:A:972:GLY:C	2:B:704:ILE:HD11	0.73	2.07	8	3
1:A:978:LEU:C	1:A:978:LEU:HD13	0.67	2.15	12	2
1:A:988:TRP:CD1	2:B:719:ILE:HD11	0.66	2.25	15	5
1:A:972:GLY:O	2:B:704:ILE:HD11	0.65	1.91	8	4
1:A:984:VAL:HG13	2:B:715:TRP:CD1	0.64	2.26	13	2
1:A:987:MET:SD	1:A:988:TRP:N	0.64	2.70	16	2
1:A:980:LEU:HD23	1:A:980:LEU:C	0.64	2.16	14	2
1:A:984:VAL:HG13	2:B:715:TRP:CG	0.62	2.29	3	2
2:B:715:TRP:CZ3	2:B:718:LEU:HD13	0.62	2.29	3	1
1:A:980:LEU:O	1:A:980:LEU:HD23	0.60	1.96	8	1
1:A:988:TRP:CD1	2:B:715:TRP:HE1	0.60	2.13	3	7
1:A:988:TRP:CD1	2:B:715:TRP:NE1	0.60	2.69	3	5
2:B:701:MET:SD	2:B:701:MET:N	0.60	2.74	10	8
1:A:983:LEU:C	1:A:987:MET:HE3	0.59	2.22	1	1
1:A:979:LEU:HD22	2:B:704:ILE:HG22	0.59	1.74	18	5
1:A:974:LEU:O	1:A:974:LEU:HD23	0.56	2.00	12	12
1:A:980:LEU:O	1:A:984:VAL:HG23	0.56	1.99	13	2
1:A:976:GLY:HA2	2:B:704:ILE:HG23	0.54	1.79	11	5
2:B:712:LEU:C	2:B:712:LEU:HD23	0.54	2.28	11	1
1:A:988:TRP:HE1	2:B:719:ILE:HD11	0.53	1.64	20	3
2:B:716:LYS:NZ	2:B:720:THR:OG1	0.53	2.41	20	1
1:A:980:LEU:HD11	1:A:984:VAL:HG23	0.51	1.83	16	1
1:A:970:LEU:O	1:A:974:LEU:N	0.51	2.42	14	19
1:A:978:LEU:HD13	1:A:978:LEU:O	0.50	2.07	1	4
1:A:974:LEU:O	1:A:974:LEU:HD13	0.50	2.07	1	2
1:A:988:TRP:HE1	2:B:719:ILE:CD1	0.48	2.21	8	11
1:A:980:LEU:O	1:A:984:VAL:CG2	0.48	2.61	13	2
1:A:988:TRP:CE2	2:B:719:ILE:HD11	0.48	2.44	12	3
1:A:987:MET:HG3	1:A:988:TRP:N	0.48	2.24	10	14
1:A:980:LEU:C	1:A:980:LEU:CD2	0.48	2.85	14	1
2:B:714:ILE:CD1	2:B:714:ILE:N	0.47	2.77	19	3
1:A:978:LEU:HD13	1:A:978:LEU:C	0.47	2.34	13	3
2:B:709:LEU:O	2:B:709:LEU:HD13	0.47	2.10	6	2
1:A:987:MET:SD	1:A:987:MET:C	0.47	2.98	8	2
2:B:718:LEU:O	2:B:718:LEU:HD13	0.47	2.10	8	3
1:A:972:GLY:O	2:B:704:ILE:CD1	0.47	2.62	8	2
2:B:708:GLY:O	2:B:712:LEU:N	0.46	2.44	12	2
1:A:974:LEU:HD23	1:A:974:LEU:C	0.46	2.35	20	5
2:B:709:LEU:O	2:B:709:LEU:HD23	0.46	2.11	15	5
1:A:985:LEU:HD13	1:A:985:LEU:O	0.46	2.10	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:987:MET:HE1	2:B:716:LYS:HA	0.46	1.87	18	2
2:B:718:LEU:HD23	2:B:718:LEU:O	0.46	2.11	13	1
1:A:974:LEU:C	1:A:974:LEU:HD23	0.46	2.36	7	1
1:A:978:LEU:C	1:A:978:LEU:CD1	0.45	2.87	12	3
2:B:705:LEU:HD23	2:B:705:LEU:O	0.45	2.12	19	14
2:B:714:ILE:N	2:B:714:ILE:HD12	0.45	2.25	19	3
1:A:988:TRP:NE1	2:B:719:ILE:CD1	0.45	2.78	11	5
1:A:972:GLY:O	2:B:704:ILE:CG1	0.44	2.65	10	3
1:A:988:TRP:CD1	2:B:719:ILE:HG23	0.44	2.47	17	2
1:A:974:LEU:HD23	1:A:974:LEU:O	0.44	2.12	7	1
1:A:988:TRP:CD1	2:B:719:ILE:CG2	0.44	3.01	1	2
2:B:718:LEU:HD13	2:B:718:LEU:C	0.43	2.37	18	1
2:B:712:LEU:C	2:B:712:LEU:CD1	0.43	2.92	16	1
1:A:987:MET:CG	1:A:988:TRP:N	0.43	2.81	8	2
1:A:972:GLY:HA3	2:B:700:VAL:HG13	0.43	1.91	16	1
1:A:980:LEU:HD23	1:A:980:LEU:O	0.42	2.12	14	1
1:A:977:LEU:HD13	1:A:977:LEU:O	0.42	2.15	7	3
2:B:717:LEU:HD12	2:B:717:LEU:N	0.42	2.29	14	1
2:B:714:ILE:N	2:B:714:ILE:CD1	0.42	2.83	17	2
2:B:718:LEU:C	2:B:718:LEU:CD1	0.42	2.92	18	1
2:B:713:LEU:O	2:B:713:LEU:HD23	0.42	2.15	17	2
1:A:984:VAL:O	1:A:987:MET:HG3	0.42	2.15	8	2
2:B:717:LEU:CD1	2:B:717:LEU:N	0.42	2.83	19	1
2:B:712:LEU:O	2:B:716:LYS:N	0.42	2.52	11	1
2:B:701:MET:N	2:B:701:MET:SD	0.42	2.93	5	1
1:A:976:GLY:O	1:A:980:LEU:N	0.41	2.43	8	2
2:B:712:LEU:O	2:B:712:LEU:HD13	0.41	2.16	16	1
2:B:713:LEU:HD23	2:B:713:LEU:O	0.41	2.16	4	2
2:B:713:LEU:HD23	2:B:713:LEU:C	0.41	2.41	4	2
1:A:988:TRP:CD1	2:B:719:ILE:CD1	0.41	3.02	15	1
2:B:717:LEU:N	2:B:717:LEU:CD2	0.41	2.83	18	1
2:B:717:LEU:N	2:B:717:LEU:CD1	0.40	2.84	10	1
1:A:975:GLY:O	1:A:979:LEU:N	0.40	2.49	16	1
2:B:713:LEU:C	2:B:713:LEU:CD2	0.40	2.95	19	1
1:A:979:LEU:HD13	1:A:979:LEU:C	0.40	2.42	6	1
2:B:712:LEU:C	2:B:712:LEU:CD2	0.40	2.95	11	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	19/54 (35%)	19±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	21/79 (27%)	21±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	800/2660 (30%)	800 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	15/44 (34%)	11±1 (70±8%)	4±1 (30±8%)	1	17
2	B	16/64 (25%)	12±1 (74±6%)	4±1 (26±6%)	2	22
All	All	620/2160 (29%)	447 (72%)	173 (28%)	1	20

All 20 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	988	TRP	20
2	B	719	ILE	19
1	A	984	VAL	18
2	B	716	LYS	18
1	A	987	MET	13
2	B	701	MET	12
2	B	705	LEU	12
1	A	983	LEU	10
1	A	970	LEU	9
1	A	974	LEU	6

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Mol	Chain	Res	Type	Models (Total)
2	B	709	LEU	6
2	B	718	LEU	5
1	A	978	LEU	4
2	B	713	LEU	4
1	A	977	LEU	4
2	B	712	LEU	4
1	A	979	LEU	3
2	B	700	VAL	3
1	A	985	LEU	2
2	B	717	LEU	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 86% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1528
Number of shifts mapped to atoms	1528
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	132	0.10 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.57 ± 0.05	Should be checked
$^{13}\text{C}'$	131	0.29 ± 0.10	None needed (< 0.5 ppm)
^{15}N	126	0.89 ± 0.10	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 86%, i.e. 511 atoms were assigned a chemical shift out of a possible 596. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	202/205 (99%)	82/85 (96%)	80/80 (100%)	40/40 (100%)
Sidechain	295/367 (80%)	207/254 (81%)	88/112 (79%)	0/1 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	14/24 (58%)	12/12 (100%)	0/10 (0%)	2/2 (100%)
Overall	511/596 (86%)	301/351 (86%)	168/202 (83%)	42/43 (98%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1528 atoms were assigned a chemical shift out of a possible 1867. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	651/668 (97%)	262/274 (96%)	263/266 (99%)	126/128 (98%)
Sidechain	828/1064 (78%)	554/701 (79%)	265/330 (80%)	9/33 (27%)
Aromatic	49/135 (36%)	44/67 (66%)	0/62 (0%)	5/6 (83%)
Overall	1528/1867 (82%)	860/1042 (83%)	528/658 (80%)	140/167 (84%)

7.1.4 Statistically unusual chemical shifts [i](#)

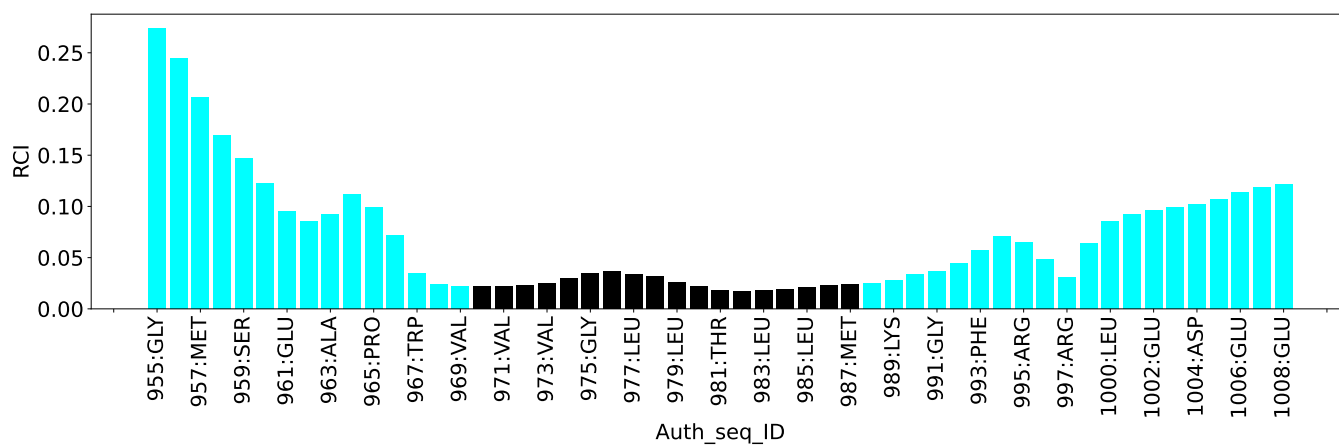
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	962	ARG	NE	110.62	76.53 – 92.65	16.1
1	A	995	ARG	NE	110.62	76.53 – 92.65	16.1
1	B	736	ARG	NE	110.44	76.53 – 92.65	16.0
1	B	734	ARG	NE	110.30	76.53 – 92.65	15.9
1	B	724	ARG	NE	110.26	76.53 – 92.65	15.9
1	A	997	ARG	CD	50.23	38.57 – 47.75	7.7

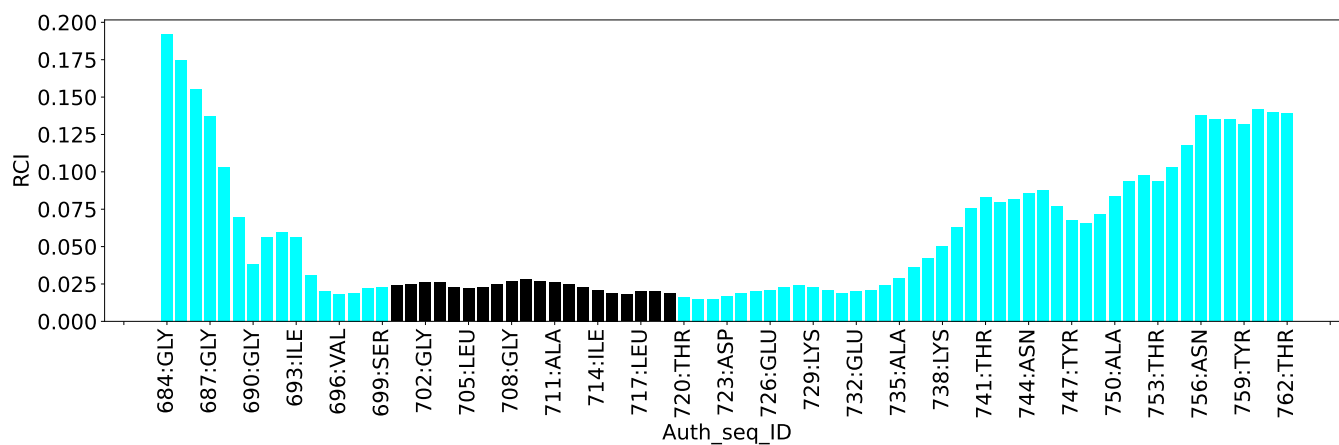
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



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	4592
Intra-residue ($ i-j =0$)	1320
Sequential ($ i-j =1$)	1306
Medium range ($ i-j >1$ and $ i-j <5$)	1484
Long range ($ i-j \geq 5$)	0
Inter-chain	164
Hydrogen bond restraints	318
Disulfide bond restraints	0
Total dihedral-angle restraints	148
Number of unmapped restraints	0
Number of restraints per residue	35.6
Number of long range restraints per residue ¹	0.0

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)	127.8	0.2
0.2-0.5 (Medium)	129.1	0.5
>0.5 (Large)	8.1	2.12

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)	10.6	9.09
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

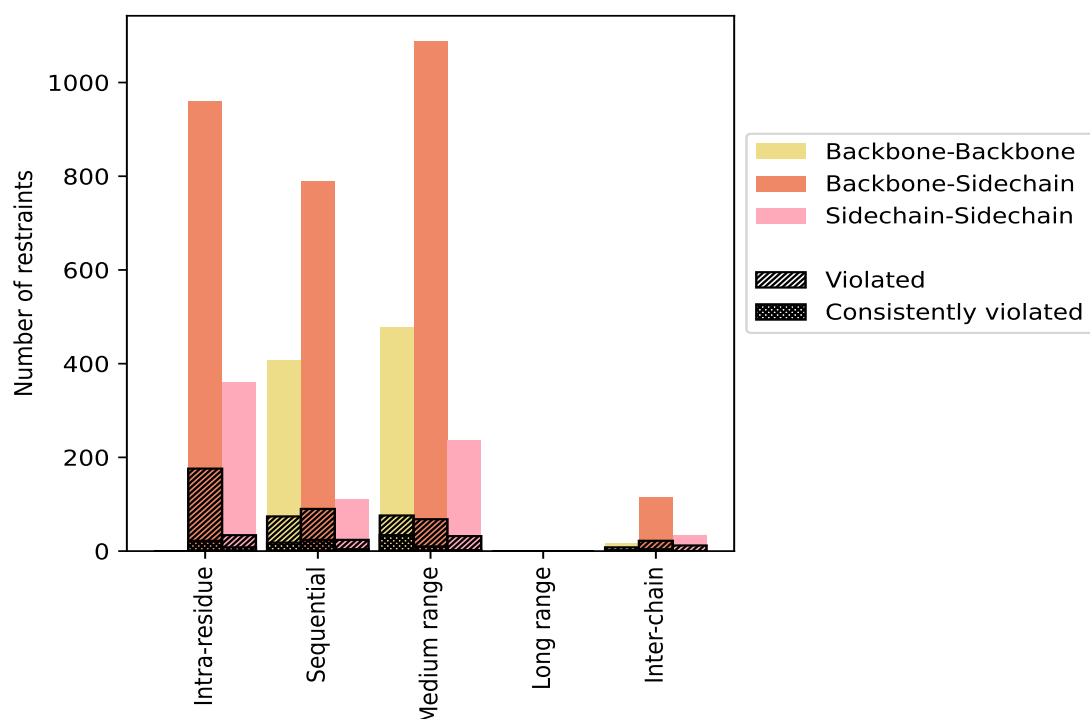
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1320	28.7	210	15.9	4.6	30	2.3	0.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	960	20.9	176	18.3	3.8	22	2.3	0.5
Sidechain-Sidechain	360	7.8	34	9.4	0.7	8	2.2	0.2
Sequential ($i-j =1$)	1306	28.4	188	14.4	4.1	46	3.5	1.0
Backbone-Backbone	406	8.8	74	18.2	1.6	18	4.4	0.4
Backbone-Sidechain	790	17.2	90	11.4	2.0	24	3.0	0.5
Sidechain-Sidechain	110	2.4	24	21.8	0.5	4	3.6	0.1
Medium range ($i-j >1$ & $i-j <5$)	1484	32.3	160	10.8	3.5	46	3.1	1.0
Backbone-Backbone	478	10.4	76	15.9	1.7	34	7.1	0.7
Backbone-Sidechain	770	16.8	52	6.8	1.1	10	1.3	0.2
Sidechain-Sidechain	236	5.1	32	13.6	0.7	2	0.8	0.0
Long range ($i-j \geq 5$)	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
Inter-chain	164	3.6	42	25.6	0.9	6	3.7	0.1
Backbone-Backbone	16	0.3	8	50.0	0.2	2	12.5	0.0
Backbone-Sidechain	114	2.5	22	19.3	0.5	4	3.5	0.1
Sidechain-Sidechain	34	0.7	12	35.3	0.3	0	0.0	0.0
Hydrogen bond	318	6.9	16	5.0	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4592	100.0	616	13.4	13.4	128	2.8	2.8
Backbone-Backbone	900	19.6	158	17.6	3.4	54	6.0	1.2
Backbone-Sidechain	2952	64.3	356	12.1	7.8	60	2.0	1.3
Sidechain-Sidechain	740	16.1	102	13.8	2.2	14	1.9	0.3

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 disulfid 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	88	90	94	0	16	288	0.24	1.05	0.13	0.2
2	88	94	86	0	18	286	0.22	0.55	0.11	0.19
3	70	80	82	0	10	242	0.25	0.76	0.13	0.21
4	82	92	80	0	16	270	0.23	0.53	0.11	0.2
5	74	94	86	0	16	270	0.24	0.79	0.12	0.2
6	74	94	86	0	22	276	0.22	0.51	0.11	0.19
7	86	86	90	0	14	276	0.25	2.12	0.2	0.21
8	82	86	96	0	18	282	0.24	1.63	0.16	0.21
9	94	90	92	0	20	296	0.22	0.58	0.11	0.19
10	78	98	82	0	18	276	0.23	0.61	0.12	0.2

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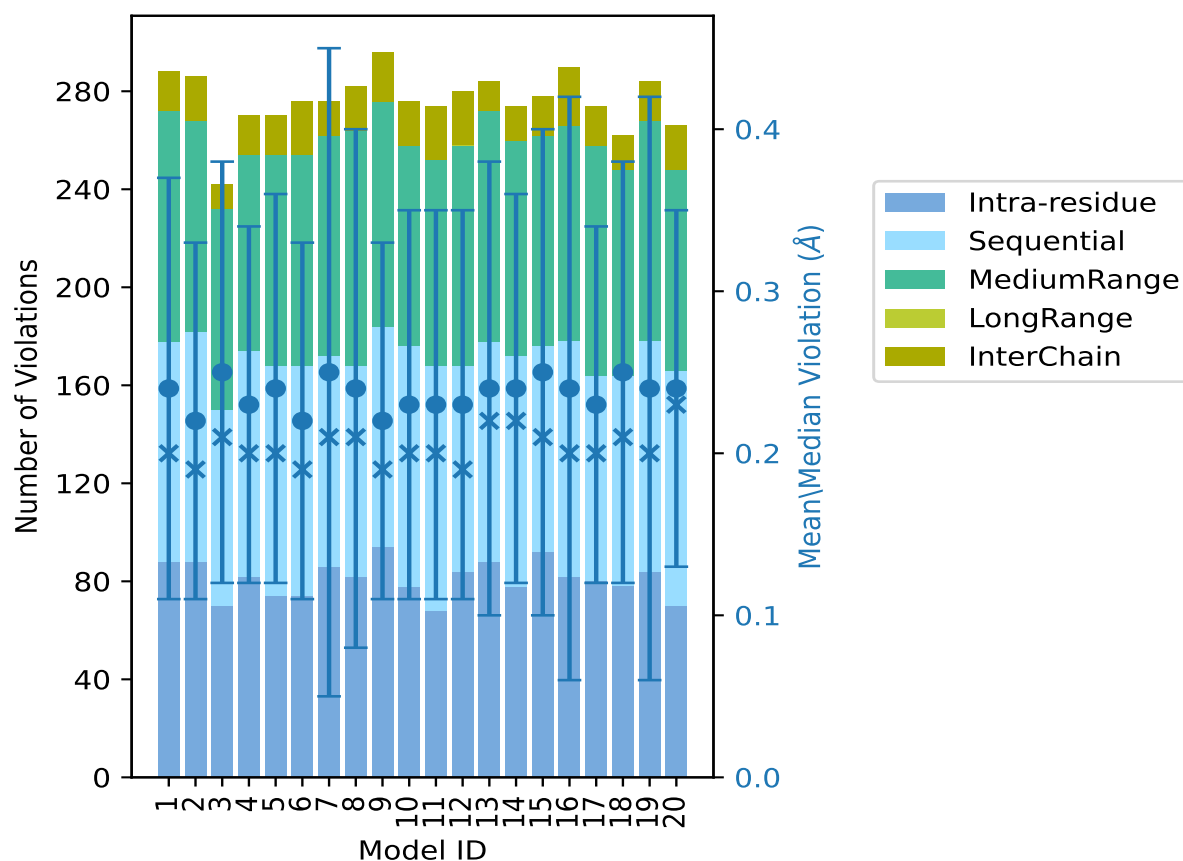
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	68	100	84	0	22	274	0.23	0.57	0.12	0.2
12	84	84	90	0	22	280	0.23	0.53	0.12	0.19
13	88	90	94	0	12	284	0.24	1.14	0.14	0.22
14	78	94	88	0	14	274	0.24	0.95	0.12	0.22
15	92	84	86	0	16	278	0.25	1.34	0.15	0.21
16	82	96	88	0	24	290	0.24	1.91	0.18	0.2
17	80	84	94	0	16	274	0.23	0.56	0.11	0.2
18	78	86	84	0	14	262	0.25	0.98	0.13	0.21
19	84	94	90	0	16	284	0.24	1.83	0.18	0.2
20	70	96	82	0	18	266	0.24	0.59	0.11	0.23

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

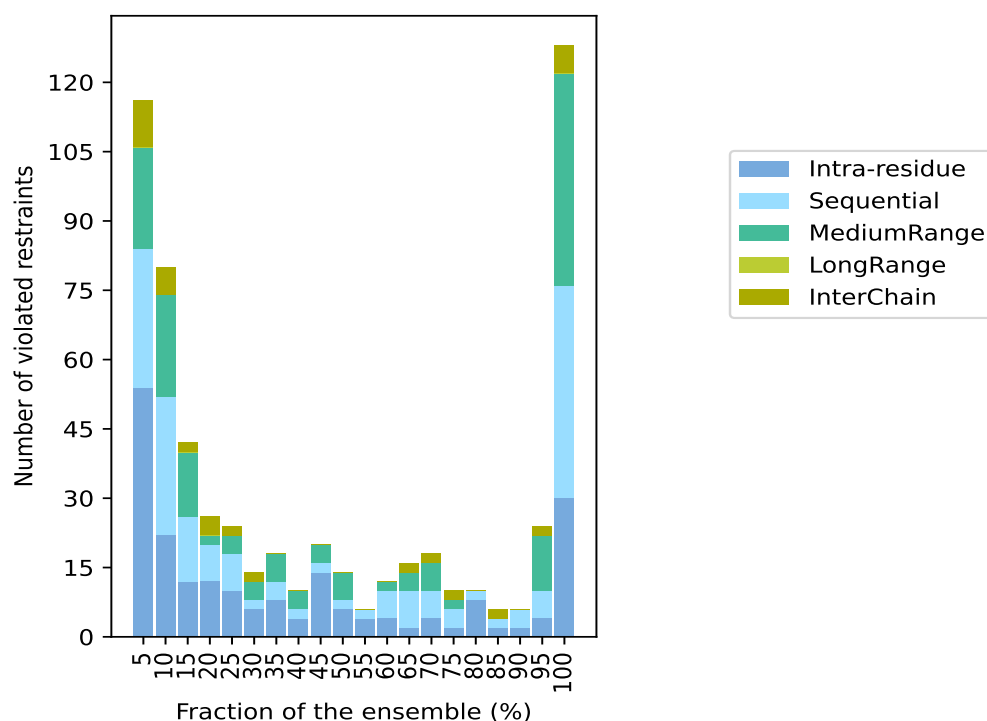
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3674(IR:1110, SQ:1118, MR:1324, LR:0, IC:122) restraints 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	%
54	30	22	0	10	116	1	5.0
22	30	22	0	6	80	2	10.0
12	14	14	0	2	42	3	15.0
12	8	2	0	4	26	4	20.0
10	8	4	0	2	24	5	25.0
6	2	4	0	2	14	6	30.0
8	4	6	0	0	18	7	35.0
4	2	4	0	0	10	8	40.0
14	2	4	0	0	20	9	45.0
6	2	6	0	0	14	10	50.0
4	2	0	0	0	6	11	55.0
4	6	2	0	0	12	12	60.0
2	8	4	0	2	16	13	65.0
4	6	6	0	2	18	14	70.0
2	4	2	0	2	10	15	75.0
8	2	0	0	0	10	16	80.0
2	2	0	0	2	6	17	85.0
2	4	0	0	0	6	18	90.0
4	6	12	0	2	24	19	95.0
30	46	46	0	6	128	20	100.0

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

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

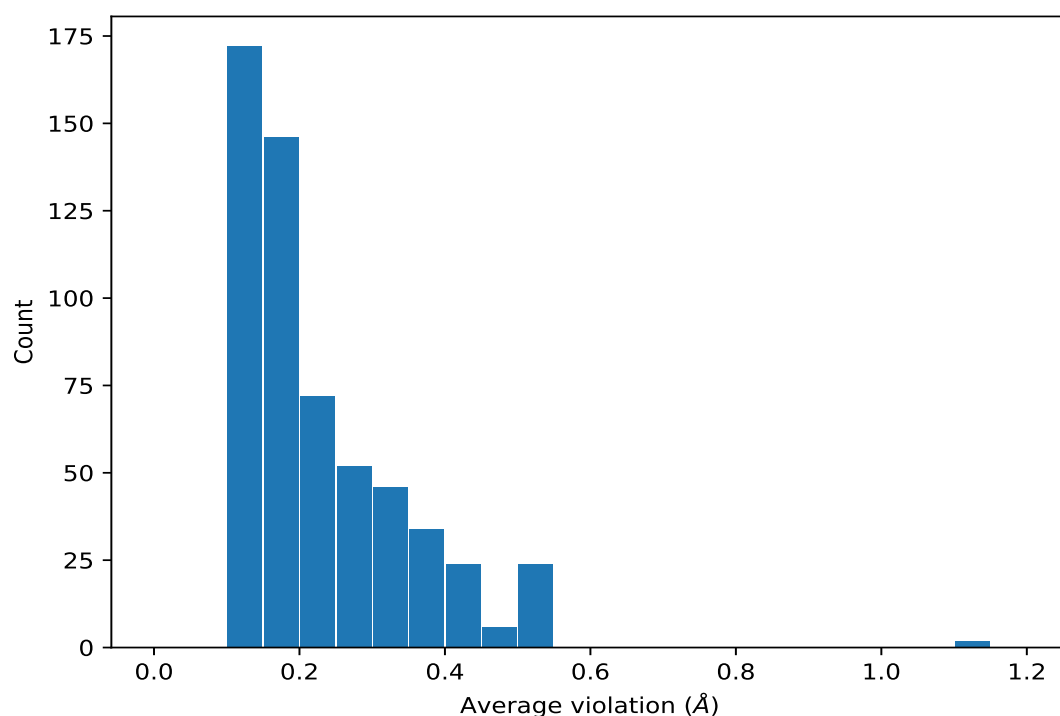
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	20	0.51	0.04	0.52
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	20	0.51	0.04	0.52
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	20	0.5	0.01	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	20	0.5	0.01	0.5
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	20	0.47	0.01	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	20	0.47	0.01	0.47
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	20	0.47	0.02	0.47
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	20	0.47	0.02	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	20	0.47	0.01	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	20	0.47	0.01	0.48
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	20	0.43	0.03	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	20	0.43	0.03	0.42
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	20	0.42	0.04	0.42
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	20	0.42	0.04	0.42
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	20	0.42	0.06	0.4
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	20	0.42	0.06	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	20	0.41	0.02	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	20	0.41	0.02	0.42
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	20	0.4	0.06	0.41
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	20	0.4	0.06	0.41
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	20	0.4	0.13	0.38
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	20	0.4	0.13	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	20	0.38	0.01	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	20	0.38	0.01	0.38
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	20	0.38	0.14	0.39
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	20	0.38	0.14	0.39
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	20	0.36	0.02	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	20	0.36	0.02	0.36
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	20	0.35	0.06	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	20	0.35	0.06	0.34
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	20	0.34	0.04	0.34
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	20	0.34	0.04	0.34
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	20	0.33	0.04	0.34
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	20	0.33	0.04	0.34
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	20	0.32	0.04	0.32
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	20	0.32	0.04	0.32
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	20	0.32	0.04	0.34
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	20	0.32	0.04	0.34
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	20	0.31	0.03	0.32
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	20	0.31	0.02	0.31
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	20	0.31	0.03	0.32
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	20	0.31	0.02	0.31
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	20	0.31	0.04	0.3
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	20	0.31	0.04	0.3
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	20	0.31	0.08	0.32
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	20	0.31	0.08	0.32
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	20	0.3	0.05	0.3
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	20	0.3	0.05	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	20	0.3	0.01	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	20	0.3	0.01	0.3
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	20	0.29	0.02	0.29
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	20	0.29	0.02	0.29
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	20	0.29	0.06	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	20	0.29	0.06	0.28
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	20	0.29	0.03	0.29
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	20	0.29	0.03	0.29
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	20	0.28	0.02	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	20	0.28	0.02	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	20	0.28	0.0	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	20	0.28	0.0	0.28
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	20	0.27	0.04	0.28
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	20	0.27	0.03	0.27
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	20	0.27	0.04	0.28
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	20	0.27	0.03	0.27
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	20	0.27	0.05	0.26
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	20	0.27	0.05	0.26
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	20	0.27	0.03	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	20	0.27	0.03	0.28
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	20	0.26	0.03	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	20	0.26	0.03	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	20	0.26	0.04	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	20	0.26	0.04	0.27
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	20	0.26	0.05	0.25
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	20	0.26	0.05	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	20	0.25	0.03	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	20	0.25	0.03	0.25
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	20	0.25	0.08	0.23
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	20	0.25	0.08	0.23
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	20	0.25	0.06	0.24
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	20	0.25	0.06	0.24
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	20	0.24	0.03	0.23
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	20	0.24	0.04	0.24
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	20	0.24	0.03	0.23
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	20	0.24	0.04	0.24
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	20	0.24	0.04	0.24
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	20	0.24	0.04	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	20	0.23	0.02	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	20	0.23	0.02	0.24
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	20	0.22	0.04	0.22
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	20	0.22	0.04	0.22
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	20	0.22	0.05	0.22
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	20	0.22	0.05	0.22
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	20	0.2	0.03	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	20	0.2	0.03	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	20	0.2	0.02	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	20	0.2	0.02	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	20	0.2	0.02	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	20	0.2	0.02	0.2
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	20	0.2	0.03	0.2
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	20	0.2	0.03	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	20	0.19	0.02	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	20	0.19	0.02	0.2
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	20	0.18	0.04	0.17
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	20	0.18	0.04	0.17
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	20	0.18	0.04	0.18
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	20	0.18	0.04	0.18
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	20	0.18	0.03	0.18
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	20	0.18	0.03	0.19
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	20	0.18	0.03	0.18
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	20	0.18	0.03	0.19
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	20	0.18	0.03	0.18
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	20	0.18	0.03	0.18
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	20	0.18	0.02	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	20	0.18	0.02	0.17
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	20	0.17	0.04	0.16
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	20	0.17	0.04	0.16
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	20	0.17	0.04	0.16
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	20	0.17	0.04	0.16
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	20	0.17	0.03	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	20	0.17	0.01	0.17
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	20	0.17	0.03	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	20	0.17	0.01	0.17
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	20	0.16	0.04	0.16
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	20	0.16	0.04	0.16
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	20	0.13	0.01	0.13
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	20	0.13	0.01	0.13
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	20	0.11	0.0	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	20	0.11	0.0	0.11
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	19	0.29	0.09	0.26
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	19	0.29	0.09	0.26
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	19	0.28	0.05	0.29
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	19	0.28	0.05	0.29
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	19	0.21	0.07	0.22
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	19	0.21	0.07	0.22
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	19	0.19	0.08	0.18
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	19	0.19	0.08	0.18
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	19	0.18	0.03	0.17
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	19	0.18	0.03	0.17
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	19	0.18	0.03	0.19
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	19	0.18	0.03	0.19
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	19	0.17	0.04	0.16
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	19	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	19	0.17	0.03	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	19	0.17	0.03	0.16
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	19	0.16	0.04	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	19	0.16	0.04	0.15
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	19	0.15	0.07	0.13
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	19	0.15	0.07	0.13
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	19	0.15	0.03	0.14
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	19	0.15	0.03	0.14
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	19	0.14	0.02	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	19	0.14	0.02	0.13
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	18	0.2	0.09	0.17
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	18	0.2	0.09	0.17
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	18	0.13	0.03	0.12
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	18	0.13	0.03	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	18	0.13	0.02	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	18	0.13	0.02	0.12
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	17	0.38	0.14	0.35
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	17	0.38	0.14	0.35
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	17	0.24	0.05	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	17	0.24	0.05	0.26
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	17	0.14	0.04	0.13
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	17	0.14	0.04	0.13
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	16	0.26	0.03	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	16	0.26	0.03	0.27
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	16	0.2	0.08	0.18
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	16	0.2	0.08	0.18
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	16	0.16	0.04	0.16
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	16	0.16	0.04	0.16
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	16	0.15	0.03	0.14
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	16	0.15	0.03	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	16	0.15	0.05	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	16	0.15	0.05	0.14
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	15	0.24	0.04	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	15	0.24	0.04	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	15	0.24	0.04	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	15	0.24	0.04	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	15	0.24	0.04	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	15	0.24	0.04	0.24
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	15	0.18	0.03	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	15	0.18	0.03	0.19
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	15	0.15	0.04	0.13
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	15	0.15	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	15	0.13	0.02	0.12
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	15	0.13	0.02	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	15	0.13	0.01	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	15	0.13	0.01	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	15	0.12	0.01	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	15	0.12	0.01	0.12
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	14	0.43	0.02	0.43
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	14	0.26	0.04	0.27
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	14	0.26	0.04	0.27
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	14	0.23	0.03	0.22
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	14	0.23	0.03	0.22
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	14	0.22	0.08	0.2
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	14	0.22	0.08	0.2
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	14	0.18	0.05	0.17
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	14	0.18	0.05	0.17
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	14	0.18	0.06	0.2
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	14	0.18	0.06	0.2
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	14	0.18	0.03	0.18
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	14	0.18	0.03	0.18
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	14	0.14	0.02	0.13
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	14	0.14	0.02	0.13
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	14	0.12	0.01	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	14	0.12	0.01	0.11
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	13	1.14	0.59	1.05
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	13	1.14	0.59	1.05
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	13	0.26	0.09	0.23
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	13	0.26	0.09	0.23
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	13	0.2	0.06	0.2
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	13	0.2	0.06	0.2
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	13	0.16	0.06	0.14
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	13	0.16	0.06	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	13	0.14	0.03	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	13	0.14	0.03	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	13	0.14	0.03	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	13	0.14	0.03	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	13	0.14	0.03	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	13	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	13	0.14	0.03	0.13
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	13	0.14	0.03	0.13
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	13	0.13	0.03	0.13
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	13	0.13	0.03	0.13
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	13	0.11	0.01	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	13	0.11	0.01	0.11
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	12	0.26	0.06	0.22
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	12	0.26	0.06	0.22
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	12	0.25	0.11	0.19
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	12	0.25	0.11	0.19
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	12	0.19	0.13	0.12
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	12	0.19	0.13	0.12
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	12	0.16	0.08	0.12
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	12	0.16	0.08	0.12
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	12	0.14	0.03	0.13
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	12	0.14	0.03	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	12	0.13	0.01	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	12	0.13	0.01	0.13
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	12	0.12	0.03	0.12
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	12	0.12	0.03	0.12
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	11	0.25	0.02	0.24
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	11	0.25	0.02	0.24
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	11	0.14	0.03	0.12
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	11	0.14	0.03	0.12
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	11	0.13	0.02	0.12
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	11	0.13	0.02	0.12
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	10	0.37	0.13	0.42
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	10	0.17	0.08	0.14
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	10	0.17	0.08	0.14
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	10	0.14	0.03	0.12
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	10	0.14	0.03	0.12
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	10	0.14	0.02	0.14
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	10	0.14	0.02	0.14
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	10	0.13	0.02	0.13
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	10	0.13	0.02	0.13
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	10	0.13	0.04	0.12
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	10	0.13	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	10	0.12	0.01	0.12
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	10	0.12	0.01	0.12
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	9	0.36	0.02	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	9	0.36	0.02	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	9	0.36	0.02	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	9	0.36	0.02	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	9	0.36	0.02	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	9	0.36	0.02	0.36
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	9	0.35	0.11	0.3
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	9	0.35	0.11	0.3
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	9	0.35	0.12	0.35
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	9	0.35	0.12	0.35
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	9	0.3	0.02	0.3
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	9	0.3	0.02	0.3
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	9	0.3	0.02	0.3
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	9	0.3	0.02	0.3
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	9	0.3	0.02	0.3
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	9	0.3	0.02	0.3
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	9	0.25	0.14	0.18
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	9	0.25	0.14	0.18
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	9	0.17	0.15	0.12
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	9	0.17	0.15	0.12
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	9	0.15	0.05	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	9	0.15	0.05	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	9	0.15	0.05	0.13
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	9	0.15	0.03	0.14
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	9	0.15	0.05	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	9	0.15	0.05	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	9	0.15	0.05	0.13
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	9	0.15	0.03	0.14
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	9	0.12	0.01	0.12
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	9	0.12	0.01	0.12
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	9	0.12	0.01	0.11
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	9	0.12	0.01	0.11
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	8	0.36	0.01	0.36
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	8	0.36	0.01	0.36
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	8	0.2	0.03	0.2
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	8	0.2	0.03	0.2
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	8	0.16	0.05	0.14
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	8	0.16	0.05	0.14
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	8	0.15	0.03	0.15
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	8	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	8	0.12	0.01	0.12
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	8	0.12	0.01	0.12
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	7	0.43	0.31	0.49
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	7	0.43	0.31	0.49
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	7	0.22	0.05	0.21
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	7	0.22	0.05	0.21
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	7	0.19	0.04	0.2
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	7	0.19	0.04	0.2
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	7	0.15	0.02	0.14
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	7	0.15	0.02	0.14
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	7	0.13	0.03	0.13
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	7	0.13	0.03	0.13
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	7	0.13	0.01	0.14
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	7	0.13	0.01	0.14
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	7	0.13	0.02	0.13
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	7	0.13	0.02	0.13
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	7	0.12	0.01	0.12
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	7	0.12	0.01	0.12
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	7	0.11	0.01	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	7	0.11	0.01	0.11
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	7	0.1	0.01	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	7	0.1	0.01	0.1
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	6	0.31	0.03	0.31
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	6	0.31	0.03	0.31
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	6	0.2	0.03	0.2
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	6	0.2	0.03	0.2
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	6	0.2	0.04	0.2
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	6	0.2	0.04	0.2
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	6	0.13	0.02	0.14
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	6	0.13	0.02	0.14
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	6	0.12	0.01	0.12
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	6	0.12	0.01	0.12
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	6	0.12	0.02	0.11
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	6	0.12	0.02	0.11
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	6	0.11	0.01	0.11
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	6	0.11	0.01	0.11
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	5	0.51	0.01	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	5	0.51	0.01	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	5	0.51	0.01	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	5	0.51	0.01	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	5	0.51	0.01	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	5	0.51	0.01	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	5	0.31	0.22	0.16
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	5	0.31	0.22	0.16
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	5	0.23	0.1	0.18
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	5	0.23	0.1	0.18
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	5	0.19	0.04	0.16
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	5	0.19	0.04	0.16
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	5	0.15	0.01	0.15
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	5	0.15	0.01	0.15
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	5	0.15	0.04	0.15
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	5	0.15	0.04	0.15
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	5	0.13	0.02	0.12
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	5	0.13	0.02	0.12
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	5	0.13	0.03	0.13
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	5	0.13	0.03	0.13
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	5	0.12	0.01	0.11
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	5	0.12	0.01	0.12
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	5	0.12	0.01	0.12
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	5	0.12	0.01	0.11
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	5	0.12	0.01	0.11
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	5	0.11	0.0	0.11
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	5	0.11	0.0	0.11
(1,1873)	2:746:B:LEU:H	2:746:B:LEU:HB3	4	0.52	0.02	0.52
(1,3956)	2:746:B:LEU:H	2:746:B:LEU:HB3	4	0.52	0.02	0.52
(1,1820)	2:742:B:ALA:HB1	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,1820)	2:742:B:ALA:HB2	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,1820)	2:742:B:ALA:HB3	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:742:B:ALA:HB1	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:742:B:ALA:HB2	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:742:B:ALA:HB3	2:743:B:ASN:H	4	0.24	0.07	0.28
(1,1957)	2:756:B:ASN:H	2:756:B:ASN:HB2	4	0.23	0.18	0.14
(1,4040)	2:756:B:ASN:H	2:756:B:ASN:HB2	4	0.23	0.18	0.14
(1,803)	1:1004:A:ASP:HA	1:1005:A:GLU:H	4	0.18	0.08	0.14
(1,2886)	1:1004:A:ASP:HA	1:1005:A:GLU:H	4	0.18	0.08	0.14
(1,801)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	4	0.16	0.09	0.12
(1,2884)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	4	0.16	0.09	0.12
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	4	0.16	0.04	0.16
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	4	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	4	0.16	0.04	0.16
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	4	0.16	0.04	0.16
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	4	0.16	0.04	0.16
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	4	0.16	0.04	0.16
(1,1811)	2:741:B:THR:HB	2:742:B:ALA:H	4	0.16	0.07	0.12
(1,3894)	2:741:B:THR:HB	2:742:B:ALA:H	4	0.16	0.07	0.12
(1,718)	1:994:A:LYS:HB2	1:995:A:ARG:H	4	0.15	0.03	0.15
(1,2801)	1:994:A:LYS:HB2	1:995:A:ARG:H	4	0.15	0.03	0.15
(1,848)	2:692:B:ASP:H	2:692:B:ASP:HB3	4	0.15	0.05	0.13
(1,2931)	2:692:B:ASP:H	2:692:B:ASP:HB3	4	0.15	0.05	0.13
(1,802)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	4	0.14	0.04	0.12
(1,2885)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	4	0.14	0.04	0.12
(1,1774)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	4	0.12	0.03	0.11
(1,3857)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	4	0.12	0.03	0.11
(1,2010)	1:969:A:VAL:HA	2:700:B:VAL:H	4	0.12	0.01	0.12
(1,4093)	1:969:A:VAL:HA	2:700:B:VAL:H	4	0.12	0.01	0.12
(1,638)	1:990:A:VAL:H	1:992:A:PHE:H	4	0.12	0.01	0.12
(1,2721)	1:990:A:VAL:H	1:992:A:PHE:H	4	0.12	0.01	0.12
(1,268)	1:974:A:LEU:HD21	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,268)	1:974:A:LEU:HD22	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,268)	1:974:A:LEU:HD23	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:974:A:LEU:HD21	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:974:A:LEU:HD22	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:974:A:LEU:HD23	1:974:A:LEU:HA	3	0.54	0.0	0.54
(1,1987)	2:759:B:TYR:H	2:759:B:TYR:HB2	3	0.41	0.21	0.55
(1,4070)	2:759:B:TYR:H	2:759:B:TYR:HB2	3	0.41	0.21	0.55
(1,1946)	2:754:B:PHE:H	2:754:B:PHE:HB3	3	0.41	0.12	0.39
(1,4029)	2:754:B:PHE:H	2:754:B:PHE:HB3	3	0.41	0.12	0.39
(1,1931)	2:751:B:THR:HA	2:752:B:SER:H	3	0.39	0.19	0.52
(1,4014)	2:751:B:THR:HA	2:752:B:SER:H	3	0.39	0.19	0.52
(1,778)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	3	0.36	0.19	0.37
(1,2861)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	3	0.36	0.19	0.37
(1,312)	1:977:A:LEU:HD11	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,312)	1:977:A:LEU:HD12	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,312)	1:977:A:LEU:HD13	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:977:A:LEU:HD11	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:977:A:LEU:HD12	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:977:A:LEU:HD13	1:977:A:LEU:HA	3	0.3	0.15	0.23
(1,1984)	2:758:B:THR:HA	2:759:B:TYR:H	3	0.28	0.0	0.28
(1,4067)	2:758:B:THR:HA	2:759:B:TYR:H	3	0.28	0.0	0.28
(1,849)	2:692:B:ASP:HB3	2:693:B:ILE:H	3	0.23	0.12	0.2
(1,2932)	2:692:B:ASP:HB3	2:693:B:ILE:H	3	0.23	0.12	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:987:A:MET:H	1:987:A:MET:HG2	3	0.2	0.03	0.21
(1,2616)	1:987:A:MET:H	1:987:A:MET:HG2	3	0.2	0.03	0.21
(1,487)	1:985:A:LEU:H	1:987:A:MET:HG2	3	0.19	0.06	0.17
(1,2570)	1:985:A:LEU:H	1:987:A:MET:HG2	3	0.19	0.06	0.17
(1,760)	1:997:A:ARG:HA	1:999:A:PRO:HD3	3	0.19	0.07	0.16
(1,2843)	1:997:A:ARG:HA	1:999:A:PRO:HD3	3	0.19	0.07	0.16
(1,740)	1:995:A:ARG:H	1:996:A:ASN:H	3	0.18	0.04	0.2
(1,2823)	1:995:A:ARG:H	1:996:A:ASN:H	3	0.18	0.04	0.2
(1,342)	1:979:A:LEU:HA	1:982:A:ILE:HB	3	0.17	0.04	0.16
(1,2425)	1:979:A:LEU:HA	1:982:A:ILE:HB	3	0.17	0.04	0.16
(1,1880)	2:746:B:LEU:HB2	2:747:B:TYR:H	3	0.17	0.03	0.17
(1,3963)	2:746:B:LEU:HB2	2:747:B:TYR:H	3	0.17	0.03	0.17
(1,1425)	2:718:B:LEU:HD21	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,1425)	2:718:B:LEU:HD22	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,1425)	2:718:B:LEU:HD23	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:718:B:LEU:HD21	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:718:B:LEU:HD22	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:718:B:LEU:HD23	2:721:B:ILE:HB	3	0.15	0.03	0.16
(1,1821)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,1821)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,1821)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	3	0.15	0.02	0.15
(1,611)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	3	0.13	0.02	0.12
(1,2694)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	3	0.13	0.02	0.12
(3,52)	1:984:A:VAL:O	1:987:A:MET:H	3	0.13	0.02	0.13
(3,211)	1:984:A:VAL:O	1:987:A:MET:H	3	0.13	0.02	0.13
(1,1273)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	3	0.12	0.01	0.13
(1,3356)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	3	0.12	0.01	0.13
(3,81)	2:700:B:VAL:O	2:704:B:ILE:H	3	0.12	0.02	0.12
(3,240)	2:700:B:VAL:O	2:704:B:ILE:H	3	0.12	0.02	0.12
(1,2002)	1:968:A:TRP:HE1	2:693:B:ILE:HB	3	0.12	0.02	0.11
(1,4085)	1:968:A:TRP:HE1	2:693:B:ILE:HB	3	0.12	0.02	0.11
(1,451)	1:984:A:VAL:H	1:987:A:MET:H	3	0.11	0.01	0.11
(1,697)	1:993:A:PHE:H	1:995:A:ARG:H	3	0.11	0.01	0.11
(1,2534)	1:984:A:VAL:H	1:987:A:MET:H	3	0.11	0.01	0.11
(1,2780)	1:993:A:PHE:H	1:995:A:ARG:H	3	0.11	0.01	0.11
(1,1380)	2:717:B:LEU:HD11	2:717:B:LEU:HA	2	0.5	0.01	0.5
(1,1380)	2:717:B:LEU:HD12	2:717:B:LEU:HA	2	0.5	0.01	0.5
(1,1380)	2:717:B:LEU:HD13	2:717:B:LEU:HA	2	0.5	0.01	0.5
(1,3463)	2:717:B:LEU:HD11	2:717:B:LEU:HA	2	0.5	0.01	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3463)	2:717:B:LEU:HD12	2:717:B:LEU:HA	2	0.5	0.01	0.5
(1,3463)	2:717:B:LEU:HD13	2:717:B:LEU:HA	2	0.5	0.01	0.5
(1,806)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	2	0.36	0.26	0.36
(1,2889)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	2	0.36	0.26	0.36
(1,776)	1:999:A:PRO:HA	1:1000:A:LEU:H	2	0.34	0.09	0.34
(1,2859)	1:999:A:PRO:HA	1:1000:A:LEU:H	2	0.34	0.09	0.34
(1,83)	1:966:A:ILE:H	1:966:A:ILE:HG12	2	0.33	0.01	0.33
(1,2166)	1:966:A:ILE:H	1:966:A:ILE:HG12	2	0.33	0.01	0.33
(1,1990)	2:759:B:TYR:HA	2:760:B:ARG:H	2	0.32	0.2	0.32
(1,4073)	2:759:B:TYR:HA	2:760:B:ARG:H	2	0.32	0.2	0.32
(1,787)	1:1000:A:LEU:HA	1:1001:A:GLU:H	2	0.32	0.1	0.32
(1,2870)	1:1000:A:LEU:HA	1:1001:A:GLU:H	2	0.32	0.1	0.32
(1,809)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	2	0.3	0.01	0.3
(1,2892)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	2	0.3	0.01	0.3
(1,1963)	2:756:B:ASN:HA	2:757:B:ILE:H	2	0.26	0.01	0.26
(1,4046)	2:756:B:ASN:HA	2:757:B:ILE:H	2	0.26	0.01	0.26
(1,1715)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	2	0.24	0.03	0.24
(1,3798)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	2	0.24	0.03	0.24
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG21	2	0.22	0.09	0.22
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG22	2	0.22	0.09	0.22
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG23	2	0.22	0.09	0.22
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG21	2	0.22	0.09	0.22
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG22	2	0.22	0.09	0.22
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG23	2	0.22	0.09	0.22
(1,869)	2:693:B:ILE:H	2:693:B:ILE:HG12	2	0.2	0.01	0.2
(1,2952)	2:693:B:ILE:H	2:693:B:ILE:HG12	2	0.2	0.01	0.2
(1,44)	1:964:A:ILE:H	1:965:A:PRO:HB2	2	0.19	0.03	0.19
(1,2127)	1:964:A:ILE:H	1:965:A:PRO:HB2	2	0.19	0.03	0.19
(1,1830)	2:743:B:ASN:H	2:743:B:ASN:HD22	2	0.18	0.01	0.18
(1,3913)	2:743:B:ASN:H	2:743:B:ASN:HD22	2	0.18	0.01	0.18
(1,488)	1:985:A:LEU:H	1:987:A:MET:HG3	2	0.18	0.06	0.18
(1,2571)	1:985:A:LEU:H	1:987:A:MET:HG3	2	0.18	0.06	0.18
(1,751)	1:996:A:ASN:H	1:997:A:ARG:H	2	0.17	0.05	0.17
(1,798)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	2	0.17	0.02	0.17
(1,813)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	2	0.17	0.02	0.17
(1,2834)	1:996:A:ASN:H	1:997:A:ARG:H	2	0.17	0.05	0.17
(1,2881)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	2	0.17	0.02	0.17
(1,2896)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	2	0.17	0.02	0.17
(1,2038)	1:976:A:GLY:H	2:707:B:ILE:HB	2	0.16	0.03	0.16
(1,2048)	1:979:A:LEU:H	2:707:B:ILE:HB	2	0.16	0.03	0.16
(1,4121)	1:976:A:GLY:H	2:707:B:ILE:HB	2	0.16	0.03	0.16
(1,4131)	1:979:A:LEU:H	2:707:B:ILE:HB	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)
(1,1658)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	2	0.15	0.03	0.15
(1,3741)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	2	0.15	0.03	0.15
(1,2055)	1:980:A:LEU:HA	2:708:B:GLY:H	2	0.15	0.04	0.15
(1,4138)	1:980:A:LEU:HA	2:708:B:GLY:H	2	0.15	0.04	0.15
(1,46)	1:964:A:ILE:HB	1:965:A:PRO:HD2	2	0.14	0.0	0.14
(1,1235)	2:709:B:LEU:HB3	2:710:B:ALA:HA	2	0.14	0.02	0.14
(1,2129)	1:964:A:ILE:HB	1:965:A:PRO:HD2	2	0.14	0.0	0.14
(1,3318)	2:709:B:LEU:HB3	2:710:B:ALA:HA	2	0.14	0.02	0.14
(1,976)	2:697:B:LEU:HB3	2:699:B:SER:H	2	0.13	0.02	0.13
(1,3059)	2:697:B:LEU:HB3	2:699:B:SER:H	2	0.13	0.02	0.13
(1,864)	2:692:B:ASP:H	2:696:B:VAL:H	2	0.12	0.01	0.12
(1,1424)	2:718:B:LEU:HD11	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,1424)	2:718:B:LEU:HD12	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,1424)	2:718:B:LEU:HD13	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,2947)	2:692:B:ASP:H	2:696:B:VAL:H	2	0.12	0.01	0.12
(1,3507)	2:718:B:LEU:HD11	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,3507)	2:718:B:LEU:HD12	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,3507)	2:718:B:LEU:HD13	2:721:B:ILE:HB	2	0.12	0.02	0.12
(1,63)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	2	0.12	0.0	0.12
(1,701)	1:993:A:PHE:HA	1:996:A:ASN:H	2	0.12	0.01	0.12
(1,1065)	2:701:B:MET:HG3	2:704:B:ILE:HG13	2	0.12	0.01	0.12
(1,2146)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	2	0.12	0.0	0.12
(1,2784)	1:993:A:PHE:HA	1:996:A:ASN:H	2	0.12	0.01	0.12
(1,3148)	2:701:B:MET:HG3	2:704:B:ILE:HG13	2	0.12	0.01	0.12
(1,313)	1:977:A:LEU:HB2	1:978:A:LEU:H	2	0.12	0.02	0.12
(1,1238)	2:709:B:LEU:HA	2:712:B:LEU:HB2	2	0.12	0.02	0.12
(1,1585)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	2	0.12	0.02	0.12
(1,2396)	1:977:A:LEU:HB2	1:978:A:LEU:H	2	0.12	0.02	0.12
(1,3321)	2:709:B:LEU:HA	2:712:B:LEU:HB2	2	0.12	0.02	0.12
(1,3668)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	2	0.12	0.02	0.12
(1,1625)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,1625)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,1625)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,1955)	2:755:B:THR:H	2:756:B:ASN:H	2	0.11	0.01	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD11	2	0.11	0.0	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD12	2	0.11	0.0	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD13	2	0.11	0.0	0.11
(1,3708)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,3708)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,3708)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	2	0.11	0.01	0.11
(1,4038)	2:755:B:THR:H	2:756:B:ASN:H	2	0.11	0.01	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD11	2	0.11	0.0	0.11

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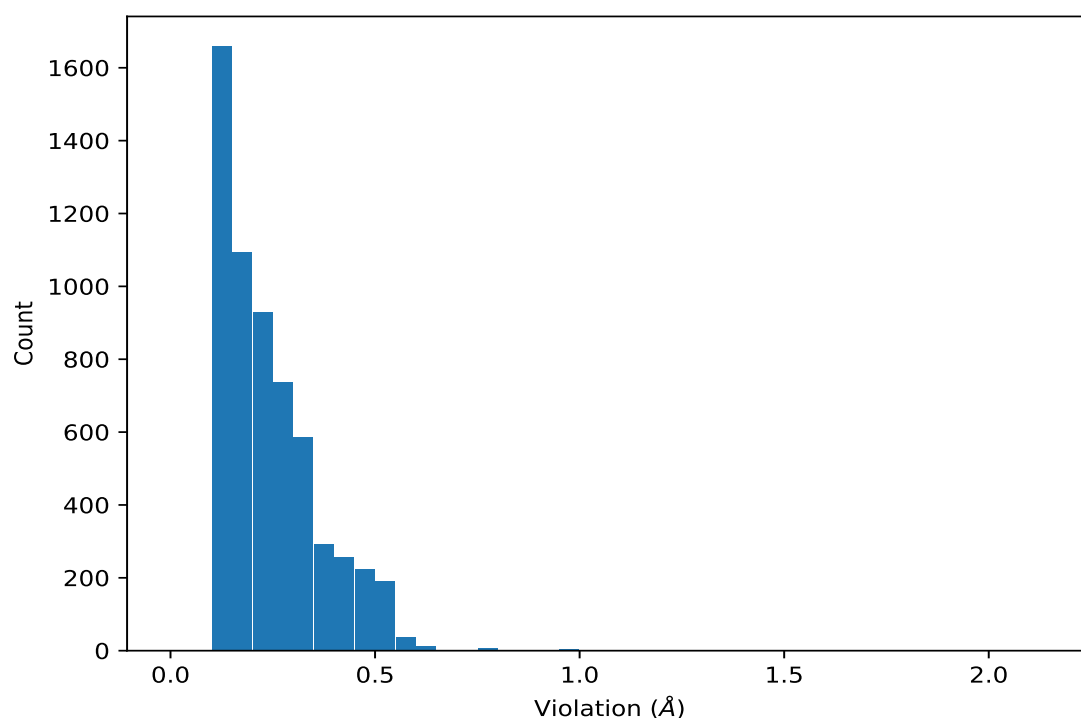
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD12	2	0.11	0.0	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD13	2	0.11	0.0	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD11	2	0.11	0.0	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD12	2	0.11	0.0	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD13	2	0.11	0.0	0.11
(1,990)	2:698:B:LEU:H	2:698:B:LEU:HB3	2	0.11	0.0	0.11
(1,1930)	2:751:B:THR:H	2:752:B:SER:H	2	0.11	0.0	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD11	2	0.11	0.0	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD12	2	0.11	0.0	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD13	2	0.11	0.0	0.11
(1,3073)	2:698:B:LEU:H	2:698:B:LEU:HB3	2	0.11	0.0	0.11
(1,4013)	2:751:B:THR:H	2:752:B:SER:H	2	0.11	0.0	0.11
(1,476)	1:985:A:LEU:HB2	1:986:A:ALA:H	2	0.1	0.0	0.1
(1,2559)	1:985:A:LEU:HB2	1:986:A:ALA:H	2	0.1	0.0	0.1
(2,27)	2:700:B:VAL:O	2:703:B:ALA:N	2	0.1	0.0	0.1
(2,81)	2:700:B:VAL:O	2:703:B:ALA:N	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	7	2.12
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	7	2.12
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	16	1.91
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	16	1.91
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	19	1.83
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	19	1.83
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	8	1.63
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	8	1.63
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	15	1.34
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	15	1.34
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	13	1.14
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	13	1.14
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	1	1.05
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	1	1.05
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	18	0.98
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	18	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	14	0.95
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	14	0.95
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	7	0.93
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	7	0.93
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	5	0.79
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	5	0.79
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	16	0.77
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	16	0.77
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	3	0.76
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	3	0.76
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	19	0.64
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	19	0.64
(1,3820)	2:736:B:ARG:H	2:736:B:ARG:HB2	15	0.62
(1,1737)	2:736:B:ARG:H	2:736:B:ARG:HB2	15	0.62
(1,2889)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	14	0.61
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	18	0.61
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	10	0.61
(1,806)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	14	0.61
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	18	0.61
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	10	0.61
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	13	0.6
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	13	0.6
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	7	0.59
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	20	0.59
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	7	0.59
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	20	0.59
(1,4070)	2:759:B:TYR:H	2:759:B:TYR:HB2	10	0.58
(1,4061)	2:757:B:ILE:HA	2:758:B:THR:H	18	0.58
(1,2861)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	9	0.58
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	13	0.58
(1,1987)	2:759:B:TYR:H	2:759:B:TYR:HB2	10	0.58
(1,1978)	2:757:B:ILE:HA	2:758:B:THR:H	18	0.58
(1,778)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	9	0.58
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	13	0.58
(1,4029)	2:754:B:PHE:H	2:754:B:PHE:HB3	11	0.57
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	1	0.57
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	14	0.57
(1,1946)	2:754:B:PHE:H	2:754:B:PHE:HB3	11	0.57
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	1	0.57
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	14	0.57
(1,3956)	2:746:B:LEU:H	2:746:B:LEU:HB3	20	0.56
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	3	0.56
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	20	0.56
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	16	0.56
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	17	0.56
(1,1873)	2:746:B:LEU:H	2:746:B:LEU:HB3	20	0.56
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	10	0.56
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	3	0.56
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	20	0.56
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	16	0.56
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	17	0.56
(1,4070)	2:759:B:TYR:H	2:759:B:TYR:HB2	9	0.55
(1,4040)	2:756:B:ASN:H	2:756:B:ASN:HB2	2	0.55
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	3	0.55
(1,1987)	2:759:B:TYR:H	2:759:B:TYR:HB2	9	0.55
(1,1957)	2:756:B:ASN:H	2:756:B:ASN:HB2	2	0.55
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	3	0.55
(1,2860)	1:1000:A:LEU:H	1:1000:A:LEU:HB2	15	0.54
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	11	0.54
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	17	0.54
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	1	0.54
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	11	0.54
(1,2351)	1:974:A:LEU:HD21	1:974:A:LEU:HA	10	0.54
(1,2351)	1:974:A:LEU:HD22	1:974:A:LEU:HA	10	0.54
(1,2351)	1:974:A:LEU:HD23	1:974:A:LEU:HA	10	0.54
(1,2351)	1:974:A:LEU:HD21	1:974:A:LEU:HA	13	0.54
(1,2351)	1:974:A:LEU:HD22	1:974:A:LEU:HA	13	0.54
(1,2351)	1:974:A:LEU:HD23	1:974:A:LEU:HA	13	0.54
(1,777)	1:1000:A:LEU:H	1:1000:A:LEU:HB2	15	0.54
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	11	0.54
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	17	0.54
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	1	0.54
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	11	0.54
(1,268)	1:974:A:LEU:HD21	1:974:A:LEU:HA	10	0.54
(1,268)	1:974:A:LEU:HD22	1:974:A:LEU:HA	10	0.54
(1,268)	1:974:A:LEU:HD23	1:974:A:LEU:HA	10	0.54
(1,268)	1:974:A:LEU:HD21	1:974:A:LEU:HA	13	0.54
(1,268)	1:974:A:LEU:HD22	1:974:A:LEU:HA	13	0.54
(1,268)	1:974:A:LEU:HD23	1:974:A:LEU:HA	13	0.54
(1,4073)	2:759:B:TYR:HA	2:760:B:ARG:H	19	0.53
(1,4014)	2:751:B:THR:HA	2:752:B:SER:H	8	0.53
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	8	0.53
(1,3956)	2:746:B:LEU:H	2:746:B:LEU:HB3	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	12	0.53
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	15	0.53
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	12	0.53
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	17	0.53
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	20	0.53
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	3	0.53
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	4	0.53
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	12	0.53
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	13	0.53
(1,2351)	1:974:A:LEU:HD21	1:974:A:LEU:HA	16	0.53
(1,2351)	1:974:A:LEU:HD22	1:974:A:LEU:HA	16	0.53
(1,2351)	1:974:A:LEU:HD23	1:974:A:LEU:HA	16	0.53
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	11	0.53
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	11	0.53
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	11	0.53
(1,1990)	2:759:B:TYR:HA	2:760:B:ARG:H	19	0.53
(1,1931)	2:751:B:THR:HA	2:752:B:SER:H	8	0.53
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	8	0.53
(1,1873)	2:746:B:LEU:H	2:746:B:LEU:HB3	13	0.53
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	12	0.53
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	15	0.53
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	12	0.53
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	17	0.53
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	20	0.53
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	3	0.53
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	4	0.53
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	12	0.53
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	13	0.53
(1,268)	1:974:A:LEU:HD21	1:974:A:LEU:HA	16	0.53
(1,268)	1:974:A:LEU:HD22	1:974:A:LEU:HA	16	0.53
(1,268)	1:974:A:LEU:HD23	1:974:A:LEU:HA	16	0.53
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	11	0.53
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	11	0.53
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	11	0.53
(1,4014)	2:751:B:THR:HA	2:752:B:SER:H	19	0.52
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	11	0.52
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	8	0.52
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	4	0.52
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	3	0.52
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	15	0.52
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	18	0.52
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	2:751:B:THR:HA	2:752:B:SER:H	19	0.52
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	11	0.52
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	8	0.52
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	4	0.52
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	3	0.52
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	15	0.52
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	18	0.52
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	12	0.52
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	18	0.51
(1,3956)	2:746:B:LEU:H	2:746:B:LEU:HB3	3	0.51
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	6	0.51
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	7	0.51
(1,3463)	2:717:B:LEU:HD11	2:717:B:LEU:HA	5	0.51
(1,3463)	2:717:B:LEU:HD12	2:717:B:LEU:HA	5	0.51
(1,3463)	2:717:B:LEU:HD13	2:717:B:LEU:HA	5	0.51
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	2	0.51
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	12	0.51
(1,2395)	1:977:A:LEU:HD11	1:977:A:LEU:HA	4	0.51
(1,2395)	1:977:A:LEU:HD12	1:977:A:LEU:HA	4	0.51
(1,2395)	1:977:A:LEU:HD13	1:977:A:LEU:HA	4	0.51
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	2	0.51
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	7	0.51
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	9	0.51
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	20	0.51
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	10	0.51
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	18	0.51
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	18	0.51
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	18	0.51
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	18	0.51
(1,1873)	2:746:B:LEU:H	2:746:B:LEU:HB3	3	0.51
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	6	0.51
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	7	0.51
(1,1380)	2:717:B:LEU:HD11	2:717:B:LEU:HA	5	0.51
(1,1380)	2:717:B:LEU:HD12	2:717:B:LEU:HA	5	0.51
(1,1380)	2:717:B:LEU:HD13	2:717:B:LEU:HA	5	0.51
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	2	0.51
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	12	0.51
(1,312)	1:977:A:LEU:HD11	1:977:A:LEU:HA	4	0.51
(1,312)	1:977:A:LEU:HD12	1:977:A:LEU:HA	4	0.51
(1,312)	1:977:A:LEU:HD13	1:977:A:LEU:HA	4	0.51
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	2	0.51
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	9	0.51
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	20	0.51
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	10	0.51
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	18	0.51
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	18	0.51
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	18	0.51
(1,3956)	2:746:B:LEU:H	2:746:B:LEU:HB3	5	0.5
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	19	0.5
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	12	0.5
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	7	0.5
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	8	0.5
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	9	0.5
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	10	0.5
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	17	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	1	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	2	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	3	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	5	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	8	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	10	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	12	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	14	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	15	0.5
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	18	0.5
(1,3463)	2:717:B:LEU:HD11	2:717:B:LEU:HA	17	0.5
(1,3463)	2:717:B:LEU:HD12	2:717:B:LEU:HA	17	0.5
(1,3463)	2:717:B:LEU:HD13	2:717:B:LEU:HA	17	0.5
(1,3079)	2:698:B:LEU:HD21	2:698:B:LEU:HA	9	0.5
(1,3079)	2:698:B:LEU:HD22	2:698:B:LEU:HA	9	0.5
(1,3079)	2:698:B:LEU:HD23	2:698:B:LEU:HA	9	0.5
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	17	0.5
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	12	0.5
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	8	0.5
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	14	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	1	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	1	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	1	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	4	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	4	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	4	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD21	20	0.5
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD22	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2269)	1:970:A:LEU:HA	1:970:A:LEU:HD23	20	0.5
(1,1873)	2:746:B:LEU:H	2:746:B:LEU:HB3	5	0.5
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	19	0.5
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	12	0.5
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	7	0.5
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	8	0.5
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	9	0.5
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	10	0.5
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	17	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	1	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	2	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	3	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	5	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	8	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	10	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	12	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	14	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	15	0.5
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	18	0.5
(1,1380)	2:717:B:LEU:HD11	2:717:B:LEU:HA	17	0.5
(1,1380)	2:717:B:LEU:HD12	2:717:B:LEU:HA	17	0.5
(1,1380)	2:717:B:LEU:HD13	2:717:B:LEU:HA	17	0.5
(1,996)	2:698:B:LEU:HD21	2:698:B:LEU:HA	9	0.5
(1,996)	2:698:B:LEU:HD22	2:698:B:LEU:HA	9	0.5
(1,996)	2:698:B:LEU:HD23	2:698:B:LEU:HA	9	0.5
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	17	0.5
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	12	0.5
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	8	0.5
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	14	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	1	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	1	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	1	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	4	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	4	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	4	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD21	20	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD22	20	0.5
(1,186)	1:970:A:LEU:HA	1:970:A:LEU:HD23	20	0.5
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	6	0.49
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	16	0.49
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	4	0.49
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	19	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	4	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	9	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	11	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	13	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	16	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	17	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	19	0.49
(1,3645)	2:725:B:LYS:H	2:725:B:LYS:HB3	20	0.49
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	6	0.49
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	1	0.49
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	5	0.49
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	10	0.49
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	14	0.49
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	3	0.49
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	3	0.49
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	3	0.49
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	5	0.49
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	5	0.49
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	5	0.49
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	6	0.49
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	6	0.49
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	6	0.49
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	9	0.49
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	9	0.49
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	9	0.49
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	15	0.49
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	15	0.49
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	15	0.49
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	6	0.49
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	16	0.49
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	4	0.49
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	13	0.49
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	19	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	4	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	9	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	11	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	13	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	16	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	17	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	19	0.49
(1,1562)	2:725:B:LYS:H	2:725:B:LYS:HB3	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	6	0.49
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	1	0.49
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	5	0.49
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	10	0.49
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	14	0.49
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	3	0.49
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	3	0.49
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	3	0.49
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	5	0.49
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	5	0.49
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	5	0.49
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	6	0.49
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	6	0.49
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	6	0.49
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	9	0.49
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	9	0.49
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	9	0.49
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	15	0.49
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	15	0.49
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	15	0.49
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	1	0.48
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	14	0.48
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	18	0.48
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	8	0.48
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	13	0.48
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	1	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	7	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	8	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	11	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	13	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	14	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	15	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	16	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	17	0.48
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	18	0.48
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	9	0.48
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	9	0.48
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	9	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	2	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	4	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	5	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	7	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	13	0.48
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	16	0.48
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	1	0.48
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	14	0.48
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	18	0.48
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	8	0.48
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	13	0.48
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	1	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	7	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	8	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	11	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	13	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	14	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	15	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	16	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	17	0.48
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	18	0.48
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	9	0.48
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	9	0.48
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	9	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	2	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	4	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	5	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	6	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	7	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	13	0.48
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	16	0.48
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	11	0.47
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	13	0.47
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	10	0.47
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	3	0.47
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	12	0.47
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	20	0.47
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	2	0.47
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	3	0.47
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	9	0.47
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	15	0.47
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	20	0.47
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	3	0.47
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	4	0.47
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	10	0.47
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	20	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	1	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	9	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	11	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	15	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	17	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	18	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	19	0.47
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	20	0.47
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	11	0.47
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	13	0.47
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	10	0.47
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	3	0.47
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	12	0.47
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	20	0.47
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	2	0.47
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	3	0.47
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	9	0.47
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	15	0.47
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	20	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	3	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	4	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	9	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	10	0.47
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	20	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	1	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	9	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	11	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	15	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	17	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	18	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	19	0.47
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	20	0.47
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	6	0.46
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	4	0.46
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	1	0.46
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	2	0.46
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	5	0.46
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	6	0.46
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	7	0.46
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	2	0.46
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	5	0.46
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	13	0.46
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	3	0.46
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	8	0.46
(1,2366)	1:975:A:GLY:HA2	1:976:A:GLY:H	10	0.46
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	6	0.46
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	4	0.46
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	1	0.46
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	2	0.46
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	5	0.46
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	6	0.46
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	7	0.46
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	4	0.46
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	2	0.46
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	5	0.46
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	13	0.46
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	3	0.46
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	8	0.46
(1,283)	1:975:A:GLY:HA2	1:976:A:GLY:H	10	0.46
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	7	0.45
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	18	0.45
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	11	0.45
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	15	0.45
(1,2883)	1:1003:A:ASP:HA	1:1004:A:ASP:H	1	0.45
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	5	0.45
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	5	0.45
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	16	0.45
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	12	0.45
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	19	0.45
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	13	0.45
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	13	0.45
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	13	0.45
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	6	0.45
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	19	0.45
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	19	0.45
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	7	0.45
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	18	0.45
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	11	0.45
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	15	0.45
(1,800)	1:1003:A:ASP:HA	1:1004:A:ASP:H	1	0.45
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	5	0.45
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	16	0.45
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	12	0.45
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	19	0.45
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	13	0.45
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	13	0.45
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	13	0.45
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	6	0.45
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	19	0.45
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	19	0.45
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	5	0.44
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	9	0.44
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	13	0.44
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	11	0.44
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	14	0.44
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	3	0.44
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	19	0.44
(1,2753)	1:992:A:PHE:HA	1:993:A:PHE:H	1	0.44
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	1	0.44
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	1	0.44
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	1	0.44
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	2	0.44
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	2	0.44
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	2	0.44
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	6	0.44
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	6	0.44
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	6	0.44
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	12	0.44
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	12	0.44
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	12	0.44
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	11	0.44
(1,2382)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	8	0.44
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	5	0.44
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	9	0.44
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	13	0.44
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	11	0.44
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	14	0.44
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	3	0.44
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	19	0.44
(1,670)	1:992:A:PHE:HA	1:993:A:PHE:H	1	0.44
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	1	0.44
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	1	0.44
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	2	0.44
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	2	0.44
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	2	0.44
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	6	0.44
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	6	0.44
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	6	0.44
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	12	0.44
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	12	0.44
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	12	0.44
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	11	0.44
(1,299)	1:976:A:GLY:HA3	1:979:A:LEU:HB3	8	0.44
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	6	0.43
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	19	0.43
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	1	0.43
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	5	0.43
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	6	0.43
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	19	0.43
(1,3435)	2:716:B:LYS:HE3	2:716:B:LYS:HG2	7	0.43
(1,2859)	1:999:A:PRO:HA	1:1000:A:LEU:H	11	0.43
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	6	0.43
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	8	0.43
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	4	0.43
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	4	0.43
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	4	0.43
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	19	0.43
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	19	0.43
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	19	0.43
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	20	0.43
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	20	0.43
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	20	0.43
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	13	0.43
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	17	0.43
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	17	0.43
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	6	0.43
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	19	0.43
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	1	0.43
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	5	0.43
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	6	0.43
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	19	0.43
(1,1352)	2:716:B:LYS:HE3	2:716:B:LYS:HG2	7	0.43
(1,776)	1:999:A:PRO:HA	1:1000:A:LEU:H	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	6	0.43
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	8	0.43
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	4	0.43
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	4	0.43
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	4	0.43
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	19	0.43
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	19	0.43
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	19	0.43
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	20	0.43
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	20	0.43
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	20	0.43
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	13	0.43
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	17	0.43
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	17	0.43
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	2	0.42
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	3	0.42
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	10	0.42
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	12	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	1	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	3	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	8	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	10	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	11	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	14	0.42
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	17	0.42
(1,2870)	1:1000:A:LEU:HA	1:1001:A:GLU:H	9	0.42
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	14	0.42
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	2	0.42
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	10	0.42
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	18	0.42
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	3	0.42
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	3	0.42
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	3	0.42
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	7	0.42
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	7	0.42
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	7	0.42
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	2	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	1	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	2	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	5	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	7	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	9	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	10	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	12	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	13	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	14	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	15	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	16	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	19	0.42
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	20	0.42
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	2	0.42
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	3	0.42
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	10	0.42
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	12	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	1	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	3	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	8	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	10	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	11	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	14	0.42
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	17	0.42
(1,787)	1:1000:A:LEU:HA	1:1001:A:GLU:H	9	0.42
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	14	0.42
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	2	0.42
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	10	0.42
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	18	0.42
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	3	0.42
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	3	0.42
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	3	0.42
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	7	0.42
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	7	0.42
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	7	0.42
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	2	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	1	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	2	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	5	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	7	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	8	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	9	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	10	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	12	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	13	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	14	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	15	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	16	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	19	0.42
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	20	0.42
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	7	0.41
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	8	0.41
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	9	0.41
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	15	0.41
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	17	0.41
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	17	0.41
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	15	0.41
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	12	0.41
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	13	0.41
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	18	0.41
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	20	0.41
(1,3715)	2:729:B:LYS:H	2:729:B:LYS:HG3	16	0.41
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	9	0.41
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	14	0.41
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	3	0.41
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	4	0.41
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	7	0.41
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	11	0.41
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	12	0.41
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	16	0.41
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	5	0.41
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	5	0.41
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	5	0.41
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	1	0.41
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	7	0.41
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	3	0.41
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	6	0.41
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	18	0.41
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	7	0.41
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	8	0.41
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	9	0.41
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	15	0.41
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	17	0.41
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	17	0.41
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	15	0.41
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	12	0.41
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	13	0.41
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	20	0.41
(1,1632)	2:729:B:LYS:H	2:729:B:LYS:HG3	16	0.41
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	9	0.41
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	14	0.41
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	3	0.41
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	4	0.41
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	7	0.41
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	11	0.41
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	12	0.41
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	16	0.41
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	5	0.41
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	5	0.41
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	5	0.41
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	1	0.41
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	7	0.41
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	3	0.41
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	6	0.41
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	18	0.41
(1,4154)	1:988:A:TRP:H	2:712:B:LEU:HD11	1	0.4
(1,4154)	1:988:A:TRP:H	2:712:B:LEU:HD12	1	0.4
(1,4154)	1:988:A:TRP:H	2:712:B:LEU:HD13	1	0.4
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	15	0.4
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	13	0.4
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	20	0.4
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	15	0.4
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	15	0.4
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	15	0.4
(1,2722)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	17	0.4
(1,2722)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	17	0.4
(1,2722)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	17	0.4
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	1	0.4
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	16	0.4
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	11	0.4
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	5	0.4
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	9	0.4
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	15	0.4
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	16	0.4
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	11	0.4
(1,2071)	1:988:A:TRP:H	2:712:B:LEU:HD11	1	0.4
(1,2071)	1:988:A:TRP:H	2:712:B:LEU:HD12	1	0.4
(1,2071)	1:988:A:TRP:H	2:712:B:LEU:HD13	1	0.4
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	13	0.4
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	20	0.4
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	15	0.4
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	15	0.4
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	15	0.4
(1,639)	1:990:A:VAL:HG11	1:992:A:PHE:HB3	17	0.4
(1,639)	1:990:A:VAL:HG12	1:992:A:PHE:HB3	17	0.4
(1,639)	1:990:A:VAL:HG13	1:992:A:PHE:HB3	17	0.4
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	1	0.4
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	16	0.4
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	11	0.4
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	5	0.4
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	9	0.4
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	15	0.4
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	16	0.4
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	11	0.4
(1,4029)	2:754:B:PHE:H	2:754:B:PHE:HB3	17	0.39
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	6	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	1	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	2	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	5	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	6	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	11	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	15	0.39
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	16	0.39
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	12	0.39
(1,2932)	2:692:B:ASP:HB3	2:693:B:ILE:H	14	0.39
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	16	0.39
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	10	0.39
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	16	0.39
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	5	0.39
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	14	0.39
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	3	0.39
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	7	0.39
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	1	0.39
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	18	0.39
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	3	0.39
(1,1946)	2:754:B:PHE:H	2:754:B:PHE:HB3	17	0.39
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	6	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	1	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	2	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	6	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	11	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	15	0.39
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	16	0.39
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	12	0.39
(1,849)	2:692:B:ASP:HB3	2:693:B:ILE:H	14	0.39
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	16	0.39
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	10	0.39
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	16	0.39
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	5	0.39
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	14	0.39
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	3	0.39
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	7	0.39
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	1	0.39
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	18	0.39
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	3	0.39
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	12	0.38
(1,3717)	2:729:B:LYS:HE3	2:729:B:LYS:HA	2	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	3	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	7	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	10	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	12	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	13	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	14	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	18	0.38
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	20	0.38
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	9	0.38
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	14	0.38
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	5	0.38
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	5	0.38
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	13	0.38
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	17	0.38
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	4	0.38
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	12	0.38
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	15	0.38
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	4	0.38
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	11	0.38
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	9	0.38
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	11	0.38
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	18	0.38
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	13	0.38
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	13	0.38
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	12	0.38
(1,1634)	2:729:B:LYS:HE3	2:729:B:LYS:HA	2	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	3	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	7	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	10	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	12	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	13	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	14	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	18	0.38
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	20	0.38
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	9	0.38
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	14	0.38
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	5	0.38
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	5	0.38
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	13	0.38
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	17	0.38
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	4	0.38
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	12	0.38
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	15	0.38
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	4	0.38
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	11	0.38
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	9	0.38
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	11	0.38
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	18	0.38
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	13	0.38
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	13	0.38
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	13	0.38
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	20	0.37
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	8	0.37
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	9	0.37
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	17	0.37
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	19	0.37
(1,2861)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	1	0.37
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	7	0.37
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	18	0.37
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	3	0.37
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	12	0.37
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	18	0.37
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	9	0.37
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	4	0.37
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	2	0.37
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	6	0.37
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	20	0.37
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	19	0.37
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	3	0.37
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	20	0.37
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	6	0.37
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	18	0.37
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	4	0.37
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	16	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	19	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	19	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	19	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	20	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	20	0.37
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	20	0.37
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	20	0.37
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	8	0.37
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	9	0.37
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	17	0.37
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	19	0.37
(1,778)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	1	0.37
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	7	0.37
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	18	0.37
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	3	0.37
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	12	0.37
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	18	0.37
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	9	0.37
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	4	0.37
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	8	0.37
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	2	0.37
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	6	0.37
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	20	0.37
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	19	0.37
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	3	0.37
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	20	0.37
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	6	0.37
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	18	0.37
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	4	0.37
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	16	0.37
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	19	0.37
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	19	0.37
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	20	0.37
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	20	0.37
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	20	0.37
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	5	0.36
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	17	0.36
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	7	0.36
(1,3713)	2:729:B:LYS:H	2:729:B:LYS:HB3	4	0.36
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	18	0.36
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	17	0.36
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	1	0.36
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	6	0.36
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	2	0.36
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	9	0.36
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	19	0.36
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	4	0.36
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	6	0.36
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	13	0.36
(1,2772)	1:993:A:PHE:HA	1:994:A:LYS:H	1	0.36
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	6	0.36
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	11	0.36
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	15	0.36
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	19	0.36
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	1	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	5	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	9	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	10	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	14	0.36
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	16	0.36
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	10	0.36
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	11	0.36
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	4	0.36
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	3	0.36
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	1	0.36
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	3	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	5	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	5	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	5	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	12	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	12	0.36
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	12	0.36
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	17	0.36
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	7	0.36
(1,1630)	2:729:B:LYS:H	2:729:B:LYS:HB3	4	0.36
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	18	0.36
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	17	0.36
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	1	0.36
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	6	0.36
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	2	0.36
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	9	0.36
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	19	0.36
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	4	0.36
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	6	0.36
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	13	0.36
(1,689)	1:993:A:PHE:HA	1:994:A:LYS:H	1	0.36
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	6	0.36
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	11	0.36
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	15	0.36
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	19	0.36
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	1	0.36
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	5	0.36
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	9	0.36
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	10	0.36
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	14	0.36
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	16	0.36
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	10	0.36
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	11	0.36
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	4	0.36
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	3	0.36
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	1	0.36
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	3	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	5	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	5	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	5	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	12	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	12	0.36
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	12	0.36
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	12	0.35
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	11	0.35
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	16	0.35
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	7	0.35
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	8	0.35
(1,2826)	1:996:A:ASN:H	1:996:A:ASN:HB3	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	15	0.35
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	1	0.35
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	17	0.35
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	11	0.35
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	14	0.35
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	10	0.35
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	5	0.35
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	17	0.35
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	17	0.35
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	19	0.35
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	10	0.35
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	16	0.35
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	17	0.35
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	19	0.35
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	19	0.35
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	19	0.35
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	8	0.35
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	18	0.35
(1,2219)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	4	0.35
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	12	0.35
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	15	0.35
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	16	0.35
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	7	0.35
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	7	0.35
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	7	0.35
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	12	0.35
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	11	0.35
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	16	0.35
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	7	0.35
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	8	0.35
(1,743)	1:996:A:ASN:H	1:996:A:ASN:HB3	15	0.35
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	15	0.35
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	1	0.35
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	17	0.35
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	11	0.35
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	14	0.35
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	10	0.35
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	5	0.35
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	17	0.35
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	17	0.35
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	19	0.35
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	16	0.35
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	17	0.35
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	19	0.35
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	19	0.35
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	19	0.35
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	8	0.35
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	18	0.35
(1,136)	1:968:A:TRP:HB3	1:968:A:TRP:HZ3	4	0.35
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	12	0.35
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	15	0.35
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	16	0.35
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	7	0.35
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	7	0.35
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	7	0.35
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	16	0.34
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	18	0.34
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	4	0.34
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	19	0.34
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	6	0.34
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	7	0.34
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	10	0.34
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	12	0.34
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	7	0.34
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	8	0.34
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	16	0.34
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	14	0.34
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	8	0.34
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	16	0.34
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	2	0.34
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	6	0.34
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	7	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	5	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	14	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	15	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	19	0.34
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	20	0.34
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	16	0.34
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	3	0.34
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	8	0.34
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	13	0.34
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	15	0.34
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	9	0.34
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	2	0.34
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	10	0.34
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	13	0.34
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	13	0.34
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	14	0.34
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	6	0.34
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	9	0.34
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	11	0.34
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	13	0.34
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	19	0.34
(1,2166)	1:966:A:ILE:H	1:966:A:ILE:HG12	15	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	1	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	1	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	1	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	8	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	8	0.34
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	8	0.34
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	16	0.34
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	18	0.34
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	4	0.34
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	19	0.34
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	6	0.34
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	7	0.34
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	10	0.34
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	12	0.34
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	7	0.34
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	8	0.34
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	16	0.34
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	14	0.34
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	8	0.34
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	16	0.34
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	2	0.34
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	6	0.34
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	7	0.34
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	5	0.34
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	14	0.34
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	15	0.34
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	19	0.34
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	20	0.34
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	16	0.34
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	8	0.34
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	13	0.34
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	15	0.34
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	18	0.34
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	9	0.34
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	2	0.34
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	10	0.34
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	13	0.34
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	13	0.34
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	14	0.34
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	6	0.34
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	9	0.34
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	11	0.34
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	13	0.34
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	19	0.34
(1,83)	1:966:A:ILE:H	1:966:A:ILE:HG12	15	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	1	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	1	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	1	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	8	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	8	0.34
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	8	0.34
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	1	0.33
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	14	0.33
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	15	0.33
(1,4069)	2:759:B:TYR:H	2:759:B:TYR:HB3	19	0.33
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	7	0.33
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	7	0.33
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	15	0.33
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	15	0.33
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	8	0.33
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	4	0.33
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	19	0.33
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	18	0.33
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	2	0.33
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	7	0.33
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	13	0.33
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	17	0.33
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	18	0.33
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	10	0.33
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	20	0.33
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	9	0.33
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	18	0.33
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	11	0.33
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	18	0.33
(1,2561)	1:985:A:LEU:HB3	1:986:A:ALA:HA	11	0.33
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	2	0.33
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	6	0.33
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	3	0.33
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	4	0.33
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	19	0.33
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	17	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	10	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	10	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	10	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	12	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	12	0.33
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	12	0.33
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	16	0.33
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	1	0.33
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	15	0.33
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	3	0.33
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	5	0.33
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	17	0.33
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD11	15	0.33
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD12	15	0.33
(1,2162)	1:966:A:ILE:HA	1:966:A:ILE:HD13	15	0.33
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	1	0.33
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	14	0.33
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	15	0.33
(1,1986)	2:759:B:TYR:H	2:759:B:TYR:HB3	19	0.33
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	7	0.33
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	7	0.33
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	15	0.33
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	15	0.33
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	8	0.33
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	4	0.33
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	19	0.33
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	18	0.33
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	2	0.33
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	7	0.33
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	13	0.33
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	18	0.33
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	10	0.33
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	20	0.33
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	4	0.33
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	9	0.33
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	18	0.33
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	11	0.33
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	18	0.33
(1,478)	1:985:A:LEU:HB3	1:986:A:ALA:HA	11	0.33
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	2	0.33
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	6	0.33
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	3	0.33
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	4	0.33
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	19	0.33
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	17	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	10	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	10	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	10	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	12	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	12	0.33
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	12	0.33
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	16	0.33
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	1	0.33
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	15	0.33
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	3	0.33
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	5	0.33
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	17	0.33
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD11	15	0.33
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD12	15	0.33
(1,79)	1:966:A:ILE:HA	1:966:A:ILE:HD13	15	0.33
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	4	0.32
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	3	0.32
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	15	0.32
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	7	0.32
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	12	0.32
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	9	0.32
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	4	0.32
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	6	0.32
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	6	0.32
(1,2886)	1:1004:A:ASP:HA	1:1005:A:GLU:H	2	0.32
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	4	0.32
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	15	0.32
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	8	0.32
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	12	0.32
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	20	0.32
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	9	0.32
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	12	0.32
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	14	0.32
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	17	0.32
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	1	0.32
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	3	0.32
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	13	0.32
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	14	0.32
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	11	0.32
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	15	0.32
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	5	0.32
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	6	0.32
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	7	0.32
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	8	0.32
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	16	0.32
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	8	0.32
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	13	0.32
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	7	0.32
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	20	0.32
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	1	0.32
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	5	0.32
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	20	0.32
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	1	0.32
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	8	0.32
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	17	0.32
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	7	0.32
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	8	0.32
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	20	0.32
(1,2166)	1:966:A:ILE:H	1:966:A:ILE:HG12	8	0.32
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	9	0.32
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	17	0.32
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	4	0.32
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	3	0.32
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	15	0.32
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	7	0.32
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	12	0.32
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	9	0.32
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	6	0.32
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	6	0.32
(1,803)	1:1004:A:ASP:HA	1:1005:A:GLU:H	2	0.32
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	4	0.32
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	10	0.32
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	15	0.32
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	8	0.32
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	12	0.32
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	20	0.32
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	9	0.32
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	12	0.32
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	14	0.32
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	17	0.32
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	1	0.32
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	3	0.32
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	13	0.32
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	14	0.32
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	11	0.32
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	15	0.32
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	5	0.32
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	6	0.32
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	7	0.32
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	8	0.32
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	16	0.32
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	8	0.32
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	13	0.32
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	7	0.32
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	20	0.32
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	1	0.32
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	5	0.32
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	20	0.32
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	1	0.32
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	8	0.32
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	17	0.32
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	7	0.32
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	8	0.32
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	20	0.32
(1,83)	1:966:A:ILE:H	1:966:A:ILE:HG12	8	0.32
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	9	0.32
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	17	0.32
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	20	0.31
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG21	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG22	15	0.31
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG23	15	0.31
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	12	0.31
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	12	0.31
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	15	0.31
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	18	0.31
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	19	0.31
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	10	0.31
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	9	0.31
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	15	0.31
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	1	0.31
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	17	0.31
(1,2892)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	13	0.31
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	11	0.31
(1,2884)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	7	0.31
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	1	0.31
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	9	0.31
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	14	0.31
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	15	0.31
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	10	0.31
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	6	0.31
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	1	0.31
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	7	0.31
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	12	0.31
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	14	0.31
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	16	0.31
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	1	0.31
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	4	0.31
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	10	0.31
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	16	0.31
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	19	0.31
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	4	0.31
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	2	0.31
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	6	0.31
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	17	0.31
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	9	0.31
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	1	0.31
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	8	0.31
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	15	0.31
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	5	0.31
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	1	0.31
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	9	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	8	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	8	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	8	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	14	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	14	0.31
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	14	0.31
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	6	0.31
(1,2282)	1:970:A:LEU:HB2	1:971:A:VAL:H	20	0.31
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	19	0.31
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	19	0.31
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	19	0.31
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	19	0.31
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	18	0.31
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	19	0.31
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	10	0.31
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	19	0.31
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	20	0.31
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG21	15	0.31
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG22	15	0.31
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG23	15	0.31
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	12	0.31
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	12	0.31
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	15	0.31
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	18	0.31
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	19	0.31
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	10	0.31
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	9	0.31
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	15	0.31
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	1	0.31
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	17	0.31
(1,809)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	13	0.31
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	11	0.31
(1,801)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	7	0.31
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	1	0.31
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	9	0.31
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	14	0.31
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	15	0.31
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	10	0.31
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	6	0.31
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	1	0.31
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	12	0.31
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	14	0.31
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	16	0.31
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	1	0.31
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	4	0.31
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	10	0.31
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	16	0.31
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	19	0.31
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	4	0.31
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	2	0.31
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	6	0.31
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	17	0.31
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	9	0.31
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	1	0.31
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	8	0.31
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	15	0.31
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	5	0.31
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	1	0.31
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	16	0.31
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	9	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	8	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	8	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	8	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	14	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	14	0.31
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	14	0.31
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	6	0.31
(1,199)	1:970:A:LEU:HB2	1:971:A:VAL:H	20	0.31
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	19	0.31
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	19	0.31
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	19	0.31
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	19	0.31
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	18	0.31
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	19	0.31
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	10	0.31
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	19	0.31
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	7	0.3
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	13	0.3
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	5	0.3
(1,3962)	2:746:B:LEU:HB3	2:747:B:TYR:H	11	0.3
(1,3903)	2:742:B:ALA:HB1	2:743:B:ASN:H	18	0.3
(1,3903)	2:742:B:ALA:HB2	2:743:B:ASN:H	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3903)	2:742:B:ALA:HB3	2:743:B:ASN:H	18	0.3
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	20	0.3
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	15	0.3
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	2	0.3
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	18	0.3
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	12	0.3
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	1	0.3
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	3	0.3
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	5	0.3
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	12	0.3
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	18	0.3
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	16	0.3
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	16	0.3
(1,2892)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	4	0.3
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	1	0.3
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	14	0.3
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	11	0.3
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	19	0.3
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	1	0.3
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	3	0.3
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	12	0.3
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	3	0.3
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	15	0.3
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	7	0.3
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	16	0.3
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	12	0.3
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	14	0.3
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	20	0.3
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	5	0.3
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	12	0.3
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	15	0.3
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	5	0.3
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	5	0.3
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	13	0.3
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	18	0.3
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	8	0.3
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	14	0.3
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	17	0.3
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	18	0.3
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	20	0.3
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	2	0.3
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	1	0.3
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	1	0.3
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	1	0.3
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	17	0.3
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	5	0.3
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	7	0.3
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	9	0.3
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	12	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	1	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	2	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	3	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	5	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	8	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	9	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	10	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	12	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	13	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	14	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	15	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	16	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	18	0.3
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	19	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	10	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	10	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	10	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	12	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	12	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	12	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	14	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	14	0.3
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	14	0.3
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	10	0.3
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	12	0.3
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	15	0.3
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	4	0.3
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	14	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	3	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	5	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	12	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	14	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	16	0.3
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	12	0.3
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	15	0.3
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	16	0.3
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	7	0.3
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	13	0.3
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	5	0.3
(1,1879)	2:746:B:LEU:HB3	2:747:B:TYR:H	11	0.3
(1,1820)	2:742:B:ALA:HB1	2:743:B:ASN:H	18	0.3
(1,1820)	2:742:B:ALA:HB2	2:743:B:ASN:H	18	0.3
(1,1820)	2:742:B:ALA:HB3	2:743:B:ASN:H	18	0.3
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	20	0.3
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	15	0.3
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	2	0.3
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	18	0.3
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	12	0.3
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	1	0.3
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	3	0.3
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	5	0.3
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	12	0.3
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	18	0.3
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	16	0.3
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	16	0.3
(1,809)	1:1005:A:GLU:HB2	1:1006:A:GLU:H	4	0.3
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	1	0.3
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	14	0.3
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	11	0.3
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	19	0.3
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	1	0.3
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	3	0.3
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	12	0.3
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	3	0.3
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	15	0.3
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	7	0.3
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	16	0.3
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	12	0.3
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	14	0.3
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	20	0.3
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	5	0.3
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	12	0.3
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	15	0.3
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	5	0.3
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	13	0.3
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	18	0.3
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	8	0.3
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	14	0.3
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	17	0.3
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	18	0.3
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	20	0.3
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	2	0.3
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	10	0.3
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	1	0.3
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	1	0.3
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	1	0.3
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	17	0.3
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	5	0.3
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	7	0.3
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	9	0.3
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	12	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	1	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	2	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	3	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	5	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	8	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	9	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	10	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	12	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	13	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	14	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	15	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	16	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	18	0.3
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	19	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	10	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	10	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	10	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	12	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	12	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	12	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	14	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	14	0.3
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	14	0.3
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	10	0.3
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	15	0.3
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	4	0.3
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	14	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	3	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	5	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	12	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	14	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	16	0.3
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	20	0.3
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	12	0.3
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	15	0.3
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	16	0.3
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	5	0.29
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	14	0.29
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	16	0.29
(1,4067)	2:758:B:THR:HA	2:759:B:TYR:H	16	0.29
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	4	0.29
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	14	0.29
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	2	0.29
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	19	0.29
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	13	0.29
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	8	0.29
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	5	0.29
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	6	0.29
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	11	0.29
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	14	0.29
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	18	0.29
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	20	0.29
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	7	0.29
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	20	0.29
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	3	0.29
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	17	0.29
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	5	0.29
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	18	0.29
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	20	0.29
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	2	0.29
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	13	0.29
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	18	0.29
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	10	0.29
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	13	0.29
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	8	0.29
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	2	0.29
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	10	0.29
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	11	0.29
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	15	0.29
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	19	0.29
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	7	0.29
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	12	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	7	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	7	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	7	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	11	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	11	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	11	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	15	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	15	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	15	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG21	16	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG22	16	0.29
(1,2446)	1:981:A:THR:H	1:981:A:THR:HG23	16	0.29
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	2	0.29
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	4	0.29
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	11	0.29
(1,2298)	1:971:A:VAL:HA	1:972:A:GLY:HA3	17	0.29
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	17	0.29
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	4	0.29
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	7	0.29
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	2	0.29
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	20	0.29
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	1	0.29
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	7	0.29
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	13	0.29
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	18	0.29
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	7	0.29
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	5	0.29
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	14	0.29
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	16	0.29
(1,1984)	2:758:B:THR:HA	2:759:B:TYR:H	16	0.29
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	4	0.29
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	14	0.29
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	2	0.29
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	19	0.29
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	8	0.29
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	5	0.29
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	6	0.29
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	11	0.29
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	14	0.29
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	18	0.29
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	20	0.29
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	7	0.29
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	20	0.29
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	3	0.29
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	17	0.29
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	5	0.29
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	18	0.29
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	20	0.29
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	2	0.29
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	13	0.29
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	18	0.29
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	10	0.29
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	13	0.29
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	8	0.29
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	13	0.29
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	2	0.29
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	10	0.29
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	11	0.29
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	15	0.29
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	19	0.29
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	7	0.29
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	12	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	7	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	7	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	7	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	11	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	11	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	11	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	15	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	15	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	15	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG21	16	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG22	16	0.29
(1,363)	1:981:A:THR:H	1:981:A:THR:HG23	16	0.29
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	2	0.29
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	11	0.29
(1,215)	1:971:A:VAL:HA	1:972:A:GLY:HA3	17	0.29
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	17	0.29
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	4	0.29
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	7	0.29
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	2	0.29
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	20	0.29
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	1	0.29
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	7	0.29
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	13	0.29
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	18	0.29
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	7	0.29
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	16	0.28
(1,4067)	2:758:B:THR:HA	2:759:B:TYR:H	11	0.28
(1,4067)	2:758:B:THR:HA	2:759:B:TYR:H	20	0.28
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	5	0.28
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	6	0.28
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	15	0.28
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	20	0.28
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	13	0.28
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	18	0.28
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	7	0.28
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	6	0.28
(1,3903)	2:742:B:ALA:HB1	2:743:B:ASN:H	7	0.28
(1,3903)	2:742:B:ALA:HB2	2:743:B:ASN:H	7	0.28
(1,3903)	2:742:B:ALA:HB3	2:743:B:ASN:H	7	0.28
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	4	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	2	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	3	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	7	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	10	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	11	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	14	0.28
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	17	0.28
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	9	0.28
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	16	0.28
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	19	0.28
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	4	0.28
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	17	0.28
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	20	0.28
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	12	0.28
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	9	0.28
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	10	0.28
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	13	0.28
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	20	0.28
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	14	0.28
(1,2945)	2:692:B:ASP:HB3	2:695:B:VAL:HA	8	0.28
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	4	0.28
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	16	0.28
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	16	0.28
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	20	0.28
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	3	0.28
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	5	0.28
(1,2843)	1:997:A:ARG:HA	1:999:A:PRO:HD3	20	0.28
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	19	0.28
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	8	0.28
(1,2707)	1:990:A:VAL:HB	1:991:A:GLY:H	11	0.28
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	3	0.28
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	15	0.28
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	5	0.28
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	15	0.28
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	5	0.28
(1,2622)	1:987:A:MET:HB3	1:988:A:TRP:H	10	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	4	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	5	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	7	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	9	0.28
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	18	0.28
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	7	0.28
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	14	0.28
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	17	0.28
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	18	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	1	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	3	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	4	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	5	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	6	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	7	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	8	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	11	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	14	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	15	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	17	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	18	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	19	0.28
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	20	0.28
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	4	0.28
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	8	0.28
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	17	0.28
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	14	0.28
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	8	0.28
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	8	0.28
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	8	0.28
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	2	0.28
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	18	0.28
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	4	0.28
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	8	0.28
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	10	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	1	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	9	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	10	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	14	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	19	0.28
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	20	0.28
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	16	0.28
(1,1984)	2:758:B:THR:HA	2:759:B:TYR:H	11	0.28
(1,1984)	2:758:B:THR:HA	2:759:B:TYR:H	20	0.28
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	5	0.28
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	6	0.28
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	15	0.28
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	20	0.28
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	13	0.28
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	18	0.28
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	7	0.28
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	6	0.28
(1,1820)	2:742:B:ALA:HB1	2:743:B:ASN:H	7	0.28
(1,1820)	2:742:B:ALA:HB2	2:743:B:ASN:H	7	0.28
(1,1820)	2:742:B:ALA:HB3	2:743:B:ASN:H	7	0.28
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	4	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	2	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	3	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	7	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	10	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	14	0.28
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	17	0.28
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	9	0.28
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	16	0.28
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	19	0.28
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	4	0.28
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	17	0.28
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	20	0.28
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	12	0.28
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	2	0.28
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	9	0.28
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	10	0.28
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	13	0.28
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	20	0.28
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	14	0.28
(1,862)	2:692:B:ASP:HB3	2:695:B:VAL:HA	8	0.28
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	4	0.28
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	16	0.28
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	16	0.28
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	20	0.28
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	3	0.28
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	5	0.28
(1,760)	1:997:A:ARG:HA	1:999:A:PRO:HD3	20	0.28
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	19	0.28
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	8	0.28
(1,624)	1:990:A:VAL:HB	1:991:A:GLY:H	11	0.28
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	3	0.28
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	15	0.28
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	5	0.28
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	15	0.28
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	5	0.28
(1,539)	1:987:A:MET:HB3	1:988:A:TRP:H	10	0.28
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	4	0.28
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	5	0.28
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	7	0.28
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	9	0.28
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	18	0.28
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	7	0.28
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	14	0.28
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	17	0.28
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	18	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	3	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	4	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	5	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	6	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	7	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	8	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	11	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	14	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	15	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	16	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	17	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	18	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	19	0.28
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	20	0.28
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	4	0.28
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	8	0.28
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	17	0.28
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	14	0.28
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	8	0.28
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	8	0.28
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	8	0.28
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	2	0.28
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	18	0.28
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	4	0.28
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	8	0.28
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	10	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	1	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	9	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	10	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	14	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	19	0.28
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	20	0.28
(1,4161)	1:988:A:TRP:H	2:719:B:ILE:HG12	20	0.27
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	18	0.27
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	8	0.27
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	7	0.27
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	8	0.27
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	13	0.27
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	16	0.27
(1,4029)	2:754:B:PHE:H	2:754:B:PHE:HB3	19	0.27
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	18	0.27
(1,3903)	2:742:B:ALA:HB1	2:743:B:ASN:H	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3903)	2:742:B:ALA:HB2	2:743:B:ASN:H	16	0.27
(1,3903)	2:742:B:ALA:HB3	2:743:B:ASN:H	16	0.27
(1,3894)	2:741:B:THR:HB	2:742:B:ALA:H	20	0.27
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	1	0.27
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	13	0.27
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	15	0.27
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	19	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	1	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	4	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	6	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	13	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	14	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	18	0.27
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	20	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	1	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	3	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	4	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	6	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	8	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	13	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	14	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	18	0.27
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	20	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	1	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	3	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	6	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	13	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	14	0.27
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	19	0.27
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	8	0.27
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	17	0.27
(1,3684)	2:726:B:GLU:HA	2:729:B:LYS:HB3	19	0.27
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	17	0.27
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	15	0.27
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	8	0.27
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	1	0.27
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	17	0.27
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	4	0.27
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	15	0.27
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	19	0.27
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	2	0.27
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	14	0.27
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	7	0.27
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	17	0.27
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	2	0.27
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	15	0.27
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	19	0.27
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	3	0.27
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	19	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	6	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	8	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	9	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	10	0.27
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	16	0.27
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	3	0.27
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	12	0.27
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	19	0.27
(1,2570)	1:985:A:LEU:H	1:987:A:MET:HG2	8	0.27
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	2	0.27
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	9	0.27
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	10	0.27
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	12	0.27
(1,2563)	1:985:A:LEU:HA	1:986:A:ALA:H	13	0.27
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	20	0.27
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	1	0.27
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	1	0.27
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	9	0.27
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	15	0.27
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	14	0.27
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	19	0.27
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	14	0.27
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	20	0.27
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	7	0.27
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	4	0.27
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	6	0.27
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	2	0.27
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	11	0.27
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	17	0.27
(1,2078)	1:988:A:TRP:H	2:719:B:ILE:HG12	20	0.27
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	18	0.27
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	8	0.27
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	7	0.27
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	13	0.27
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	16	0.27
(1,1946)	2:754:B:PHE:H	2:754:B:PHE:HB3	19	0.27
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	18	0.27
(1,1820)	2:742:B:ALA:HB1	2:743:B:ASN:H	16	0.27
(1,1820)	2:742:B:ALA:HB2	2:743:B:ASN:H	16	0.27
(1,1820)	2:742:B:ALA:HB3	2:743:B:ASN:H	16	0.27
(1,1811)	2:741:B:THR:HB	2:742:B:ALA:H	20	0.27
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	1	0.27
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	13	0.27
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	15	0.27
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	19	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	1	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	4	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	6	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	13	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	14	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	18	0.27
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	20	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	1	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	3	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	4	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	6	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	8	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	13	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	14	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	18	0.27
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	20	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	1	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	3	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	6	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	13	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	14	0.27
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	19	0.27
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	8	0.27
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	17	0.27
(1,1601)	2:726:B:GLU:HA	2:729:B:LYS:HB3	19	0.27
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	17	0.27
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	15	0.27
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	8	0.27
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	1	0.27
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	4	0.27
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	15	0.27
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	19	0.27
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	2	0.27
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	3	0.27
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	14	0.27
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	7	0.27
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	17	0.27
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	2	0.27
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	15	0.27
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	19	0.27
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	3	0.27
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	19	0.27
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	6	0.27
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	8	0.27
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	9	0.27
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	10	0.27
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	16	0.27
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	3	0.27
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	12	0.27
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	19	0.27
(1,487)	1:985:A:LEU:H	1:987:A:MET:HG2	8	0.27
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	2	0.27
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	9	0.27
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	10	0.27
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	12	0.27
(1,480)	1:985:A:LEU:HA	1:986:A:ALA:H	13	0.27
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	20	0.27
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	1	0.27
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	1	0.27
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	9	0.27
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	15	0.27
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	14	0.27
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	19	0.27
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	14	0.27
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	20	0.27
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	7	0.27
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	4	0.27
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	6	0.27
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	2	0.27
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	11	0.27
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	2	0.26
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	20	0.26
(1,4046)	2:756:B:ASN:HA	2:757:B:ILE:H	11	0.26
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	18	0.26
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	7	0.26
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	1	0.26
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	2	0.26
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	12	0.26
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	14	0.26
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	15	0.26
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	13	0.26
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	17	0.26
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	1	0.26
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	19	0.26
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	11	0.26
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	5	0.26
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	6	0.26
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	9	0.26
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	18	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	3	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	8	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	9	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	16	0.26
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	19	0.26
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	16	0.26
(1,3798)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	2	0.26
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	11	0.26
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	18	0.26
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	19	0.26
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	12	0.26
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	16	0.26
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	6	0.26
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	16	0.26
(1,2789)	1:994:A:LYS:H	1:994:A:LYS:HB3	9	0.26
(1,2685)	1:989:A:LYS:HA	1:991:A:GLY:H	6	0.26
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	20	0.26
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	9	0.26
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	14	0.26
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	19	0.26
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	11	0.26
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	6	0.26
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	6	0.26
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	2	0.26
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	20	0.26
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	9	0.26
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	14	0.26
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	11	0.26
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	15	0.26
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	18	0.26
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	17	0.26
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	1	0.26
(1,2499)	1:983:A:LEU:HB2	1:984:A:VAL:H	14	0.26
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	5	0.26
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	11	0.26
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	8	0.26
(1,2368)	1:975:A:GLY:HA3	1:977:A:LEU:H	6	0.26
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	6	0.26
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	11	0.26
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	2	0.26
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	3	0.26
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	11	0.26
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	15	0.26
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	4	0.26
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	5	0.26
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	6	0.26
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	13	0.26
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	2	0.26
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	20	0.26
(1,1963)	2:756:B:ASN:HA	2:757:B:ILE:H	11	0.26
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	18	0.26
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	7	0.26
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	1	0.26
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	2	0.26
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	12	0.26
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	14	0.26
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	15	0.26
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	13	0.26
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	17	0.26
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	1	0.26
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	19	0.26
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	11	0.26
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	5	0.26
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	9	0.26
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	18	0.26
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	3	0.26
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	8	0.26
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	9	0.26
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	16	0.26
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	19	0.26
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	16	0.26
(1,1715)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	2	0.26
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	11	0.26
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	18	0.26
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	19	0.26
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	12	0.26
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	16	0.26
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	6	0.26
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	16	0.26
(1,706)	1:994:A:LYS:H	1:994:A:LYS:HB3	9	0.26
(1,602)	1:989:A:LYS:HA	1:991:A:GLY:H	6	0.26
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	20	0.26
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	9	0.26
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	14	0.26
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	19	0.26
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	11	0.26
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	6	0.26
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	16	0.26
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	6	0.26
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	2	0.26
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	20	0.26
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	9	0.26
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	14	0.26
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	11	0.26
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	15	0.26
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	18	0.26
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	17	0.26
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	1	0.26
(1,416)	1:983:A:LEU:HB2	1:984:A:VAL:H	14	0.26
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	5	0.26
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	11	0.26
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	8	0.26
(1,285)	1:975:A:GLY:HA3	1:977:A:LEU:H	6	0.26
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	6	0.26
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	2	0.26
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	3	0.26
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	11	0.26
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	15	0.26
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	4	0.26
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	5	0.26
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	6	0.26
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	13	0.26
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	6	0.25
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	14	0.25
(1,4046)	2:756:B:ASN:HA	2:757:B:ILE:H	2	0.25
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	1	0.25
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	20	0.25
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	5	0.25
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	6	0.25
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	13	0.25
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	14	0.25
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	8	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	1	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	4	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	5	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	6	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	12	0.25
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	19	0.25
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	2	0.25
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	10	0.25
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	13	0.25
(1,2929)	2:691:B:PRO:HA	2:692:B:ASP:HB3	8	0.25
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	5	0.25
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	11	0.25
(1,2859)	1:999:A:PRO:HA	1:1000:A:LEU:H	6	0.25
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	11	0.25
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	2	0.25
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	4	0.25
(1,2806)	1:994:A:LYS:HD3	1:995:A:ARG:H	20	0.25
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	16	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	4	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	6	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	7	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	11	0.25
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	13	0.25
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	2	0.25
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	6	0.25
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	12	0.25
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	12	0.25
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	3	0.25
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	5	0.25
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	7	0.25
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	17	0.25
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	20	0.25
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	3	0.25
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	15	0.25
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	8	0.25
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	15	0.25
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	18	0.25
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	4	0.25
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	13	0.25
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	18	0.25
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	9	0.25
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	1	0.25
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	2	0.25
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	18	0.25
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	8	0.25
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	6	0.25
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	14	0.25
(1,1963)	2:756:B:ASN:HA	2:757:B:ILE:H	2	0.25
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	1	0.25
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	20	0.25
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	5	0.25
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	6	0.25
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	13	0.25
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	14	0.25
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	8	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	1	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	4	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	5	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	6	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	12	0.25
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	19	0.25
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	2	0.25
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	10	0.25
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	13	0.25
(1,846)	2:691:B:PRO:HA	2:692:B:ASP:HB3	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	5	0.25
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	11	0.25
(1,776)	1:999:A:PRO:HA	1:1000:A:LEU:H	6	0.25
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	11	0.25
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	2	0.25
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	4	0.25
(1,723)	1:994:A:LYS:HD3	1:995:A:ARG:H	20	0.25
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	16	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	4	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	6	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	7	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	11	0.25
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	13	0.25
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	7	0.25
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	2	0.25
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	6	0.25
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	12	0.25
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	12	0.25
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	3	0.25
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	5	0.25
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	7	0.25
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	17	0.25
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	20	0.25
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	3	0.25
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	15	0.25
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	8	0.25
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	15	0.25
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	18	0.25
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	4	0.25
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	13	0.25
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	18	0.25
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	9	0.25
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	1	0.25
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	2	0.25
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	18	0.25
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	8	0.25
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	8	0.24
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	1	0.24
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	10	0.24
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	17	0.24
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	19	0.24
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	3	0.24
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	9	0.24
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	17	0.24
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	17	0.24
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	1	0.24
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	5	0.24
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	2	0.24
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	19	0.24
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	1	0.24
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	10	0.24
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	3	0.24
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	2	0.24
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	20	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	2	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	3	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	10	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	14	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	17	0.24
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	20	0.24
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	8	0.24
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	6	0.24
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	14	0.24
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	13	0.24
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	13	0.24
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	13	0.24
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	9	0.24
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	10	0.24
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	16	0.24
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	14	0.24
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	1	0.24
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	2	0.24
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	16	0.24
(1,2660)	1:989:A:LYS:H	1:989:A:LYS:HB3	19	0.24
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	9	0.24
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	14	0.24
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	10	0.24
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	11	0.24
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	1	0.24
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	3	0.24
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	4	0.24
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	13	0.24
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	20	0.24
(1,2571)	1:985:A:LEU:H	1:987:A:MET:HG3	1	0.24
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	16	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	3	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	3	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	3	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	13	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	13	0.24
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	13	0.24
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	13	0.24
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	2	0.24
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	3	0.24
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	13	0.24
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	20	0.24
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	3	0.24
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	6	0.24
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	13	0.24
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	7	0.24
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	11	0.24
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	8	0.24
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	8	0.24
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	8	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	1	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	1	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	1	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	4	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	4	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	4	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	18	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	18	0.24
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	18	0.24
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	7	0.24
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	10	0.24
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	16	0.24
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	18	0.24
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	10	0.24
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	16	0.24
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	17	0.24
(1,2088)	1:960:A:GLU:HA	1:961:A:GLU:H	18	0.24
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	8	0.24
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	1	0.24
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	17	0.24
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	19	0.24
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	10	0.24
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	3	0.24
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	9	0.24
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	17	0.24
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	17	0.24
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	1	0.24
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	5	0.24
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	2	0.24
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	19	0.24
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	1	0.24
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	10	0.24
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	3	0.24
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	2	0.24
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	20	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	2	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	3	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	10	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	14	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	17	0.24
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	20	0.24
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	8	0.24
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	6	0.24
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	14	0.24
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	13	0.24
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	13	0.24
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	13	0.24
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	9	0.24
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	10	0.24
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	16	0.24
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	14	0.24
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	1	0.24
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	2	0.24
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	16	0.24
(1,577)	1:989:A:LYS:H	1:989:A:LYS:HB3	19	0.24
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	9	0.24
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	14	0.24
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	10	0.24
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	11	0.24
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	1	0.24
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	4	0.24
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	13	0.24
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	7	0.24
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	20	0.24
(1,488)	1:985:A:LEU:H	1:987:A:MET:HG3	1	0.24
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	16	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	3	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	3	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	3	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	13	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	13	0.24
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	13	0.24
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	13	0.24
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	2	0.24
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	3	0.24
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	13	0.24
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	20	0.24
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	3	0.24
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	6	0.24
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	13	0.24
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	7	0.24
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	11	0.24
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	8	0.24
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	8	0.24
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	8	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	1	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	1	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	1	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	4	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	4	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	4	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	18	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	18	0.24
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	18	0.24
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	7	0.24
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	10	0.24
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	16	0.24
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	18	0.24
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	10	0.24
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	16	0.24
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	17	0.24
(1,5)	1:960:A:GLU:HA	1:961:A:GLU:H	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	7	0.23
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	7	0.23
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	8	0.23
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	9	0.23
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	9	0.23
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	2	0.23
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	4	0.23
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	15	0.23
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	4	0.23
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	14	0.23
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	16	0.23
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	13	0.23
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	20	0.23
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	11	0.23
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	20	0.23
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	13	0.23
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	13	0.23
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	11	0.23
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	13	0.23
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	16	0.23
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	8	0.23
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	1	0.23
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	19	0.23
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	16	0.23
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	3	0.23
(1,2931)	2:692:B:ASP:H	2:692:B:ASP:HB3	8	0.23
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	20	0.23
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	5	0.23
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	6	0.23
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	17	0.23
(1,2824)	1:995:A:ARG:HB3	1:997:A:ARG:H	5	0.23
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	18	0.23
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	1	0.23
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	11	0.23
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	8	0.23
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	17	0.23
(1,2616)	1:987:A:MET:H	1:987:A:MET:HG2	8	0.23
(1,2602)	1:986:A:ALA:HA	1:989:A:LYS:H	8	0.23
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	4	0.23
(1,2599)	1:986:A:ALA:HA	1:988:A:TRP:H	20	0.23
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	4	0.23
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	13	0.23
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	18	0.23
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	13	0.23
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	7	0.23
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	15	0.23
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	10	0.23
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	1	0.23
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	7	0.23
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	15	0.23
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	20	0.23
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	14	0.23
(1,2425)	1:979:A:LEU:HA	1:982:A:ILE:HB	12	0.23
(1,2395)	1:977:A:LEU:HD11	1:977:A:LEU:HA	14	0.23
(1,2395)	1:977:A:LEU:HD12	1:977:A:LEU:HA	14	0.23
(1,2395)	1:977:A:LEU:HD13	1:977:A:LEU:HA	14	0.23
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	20	0.23
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	12	0.23
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	12	0.23
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	12	0.23
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	20	0.23
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	20	0.23
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	20	0.23
(1,2224)	1:968:A:TRP:HB2	1:969:A:VAL:H	12	0.23
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	14	0.23
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	6	0.23
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	16	0.23
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	9	0.23
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	14	0.23
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	17	0.23
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	7	0.23
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	7	0.23
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	8	0.23
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	9	0.23
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	9	0.23
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	2	0.23
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	4	0.23
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	15	0.23
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	4	0.23
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	14	0.23
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	16	0.23
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	13	0.23
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	11	0.23
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	20	0.23
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	13	0.23
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	13	0.23
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	11	0.23
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	13	0.23
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	16	0.23
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	8	0.23
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	1	0.23
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	19	0.23
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	16	0.23
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	3	0.23
(1,848)	2:692:B:ASP:H	2:692:B:ASP:HB3	8	0.23
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	20	0.23
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	5	0.23
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	6	0.23
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	17	0.23
(1,741)	1:995:A:ARG:HB3	1:997:A:ARG:H	5	0.23
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	18	0.23
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	1	0.23
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	11	0.23
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	8	0.23
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	17	0.23
(1,533)	1:987:A:MET:H	1:987:A:MET:HG2	8	0.23
(1,519)	1:986:A:ALA:HA	1:989:A:LYS:H	8	0.23
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	4	0.23
(1,516)	1:986:A:ALA:HA	1:988:A:TRP:H	20	0.23
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	4	0.23
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	10	0.23
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	13	0.23
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	18	0.23
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	13	0.23
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	7	0.23
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	15	0.23
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	10	0.23
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	1	0.23
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	7	0.23
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	15	0.23
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	20	0.23
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	14	0.23
(1,342)	1:979:A:LEU:HA	1:982:A:ILE:HB	12	0.23
(1,312)	1:977:A:LEU:HD11	1:977:A:LEU:HA	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:977:A:LEU:HD12	1:977:A:LEU:HA	14	0.23
(1,312)	1:977:A:LEU:HD13	1:977:A:LEU:HA	14	0.23
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	20	0.23
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	12	0.23
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	12	0.23
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	12	0.23
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	20	0.23
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	20	0.23
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	20	0.23
(1,141)	1:968:A:TRP:HB2	1:969:A:VAL:H	12	0.23
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	14	0.23
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	6	0.23
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	16	0.23
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	9	0.23
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	14	0.23
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	17	0.23
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	15	0.22
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	15	0.22
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	15	0.22
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	12	0.22
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	14	0.22
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	6	0.22
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	10	0.22
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	19	0.22
(1,4077)	2:760:B:ARG:H	2:760:B:ARG:HB2	9	0.22
(1,4004)	2:749:B:GLU:HB2	2:750:B:ALA:H	10	0.22
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	14	0.22
(1,3998)	2:749:B:GLU:H	2:749:B:GLU:HB3	15	0.22
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	4	0.22
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	11	0.22
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	4	0.22
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	8	0.22
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	11	0.22
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	9	0.22
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	2	0.22
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	17	0.22
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	11	0.22
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	13	0.22
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	13	0.22
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	14	0.22
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	10	0.22
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	5	0.22
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	8	0.22
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	9	0.22
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	8	0.22
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	10	0.22
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	13	0.22
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	15	0.22
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	14	0.22
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	6	0.22
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	2	0.22
(1,2870)	1:1000:A:LEU:HA	1:1001:A:GLU:H	16	0.22
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	18	0.22
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	12	0.22
(1,2834)	1:996:A:ASN:H	1:997:A:ARG:H	5	0.22
(1,2823)	1:995:A:ARG:H	1:996:A:ASN:H	18	0.22
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	20	0.22
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	19	0.22
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	10	0.22
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	9	0.22
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	10	0.22
(1,2673)	1:989:A:LYS:HB2	1:990:A:VAL:H	12	0.22
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	12	0.22
(1,2582)	1:985:A:LEU:HA	1:989:A:LYS:H	17	0.22
(1,2572)	1:985:A:LEU:HA	1:988:A:TRP:H	17	0.22
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	4	0.22
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	11	0.22
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	16	0.22
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	5	0.22
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	20	0.22
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	5	0.22
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	9	0.22
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	9	0.22
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	11	0.22
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	14	0.22
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	19	0.22
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	18	0.22
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	16	0.22
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	14	0.22
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	1	0.22
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	14	0.22
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	14	0.22
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	10	0.22
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	10	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	3	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	3	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	3	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	5	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	5	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	5	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	9	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	9	0.22
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	9	0.22
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	4	0.22
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	9	0.22
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	13	0.22
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	12	0.22
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	13	0.22
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	17	0.22
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	19	0.22
(1,2164)	1:966:A:ILE:H	1:966:A:ILE:HG13	11	0.22
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	2	0.22
(1,2128)	1:964:A:ILE:HB	1:965:A:PRO:HD3	6	0.22
(1,2127)	1:964:A:ILE:H	1:965:A:PRO:HB2	13	0.22
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	12	0.22
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	15	0.22
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	15	0.22
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	15	0.22
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	12	0.22
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	14	0.22
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	6	0.22
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	10	0.22
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	19	0.22
(1,1994)	2:760:B:ARG:H	2:760:B:ARG:HB2	9	0.22
(1,1921)	2:749:B:GLU:HB2	2:750:B:ALA:H	10	0.22
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	14	0.22
(1,1915)	2:749:B:GLU:H	2:749:B:GLU:HB3	15	0.22
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	4	0.22
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	11	0.22
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	4	0.22
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	8	0.22
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	11	0.22
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	9	0.22
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	17	0.22
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	11	0.22
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	13	0.22
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	13	0.22
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	14	0.22
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	10	0.22
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	17	0.22
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	5	0.22
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	8	0.22
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	9	0.22
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	8	0.22
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	10	0.22
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	13	0.22
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	15	0.22
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	14	0.22
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	6	0.22
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	2	0.22
(1,787)	1:1000:A:LEU:HA	1:1001:A:GLU:H	16	0.22
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	18	0.22
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	12	0.22
(1,751)	1:996:A:ASN:H	1:997:A:ARG:H	5	0.22
(1,740)	1:995:A:ARG:H	1:996:A:ASN:H	18	0.22
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	20	0.22
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	19	0.22
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	10	0.22
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	9	0.22
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	10	0.22
(1,590)	1:989:A:LYS:HB2	1:990:A:VAL:H	12	0.22
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	12	0.22
(1,499)	1:985:A:LEU:HA	1:989:A:LYS:H	17	0.22
(1,489)	1:985:A:LEU:HA	1:988:A:TRP:H	17	0.22
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	4	0.22
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	11	0.22
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	16	0.22
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	5	0.22
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	20	0.22
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	5	0.22
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	9	0.22
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	9	0.22
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	11	0.22
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	14	0.22
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	18	0.22
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	16	0.22
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	14	0.22
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	1	0.22
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	14	0.22
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	14	0.22
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	10	0.22
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	10	0.22
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	10	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	3	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	3	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	3	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	5	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	5	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	5	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	9	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	9	0.22
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	9	0.22
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	4	0.22
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	9	0.22
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	13	0.22
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	12	0.22
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	13	0.22
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	17	0.22
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	19	0.22
(1,81)	1:966:A:ILE:H	1:966:A:ILE:HG13	11	0.22
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	2	0.22
(1,45)	1:964:A:ILE:HB	1:965:A:PRO:HD3	6	0.22
(1,44)	1:964:A:ILE:H	1:965:A:PRO:HB2	13	0.22
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	12	0.22
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	16	0.21
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	16	0.21
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	15	0.21
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	15	0.21
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	15	0.21
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	6	0.21
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	11	0.21
(1,4102)	1:973:A:VAL:H	2:701:B:MET:HE1	16	0.21
(1,4102)	1:973:A:VAL:H	2:701:B:MET:HE2	16	0.21
(1,4102)	1:973:A:VAL:H	2:701:B:MET:HE3	16	0.21
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	19	0.21
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	9	0.21
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	10	0.21
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	8	0.21
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	9	0.21
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	14	0.21
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	16	0.21
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	7	0.21
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	18	0.21
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	3	0.21
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	13	0.21
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	14	0.21
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	9	0.21
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	8	0.21
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	9	0.21
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	5	0.21
(1,3859)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	10	0.21
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	7	0.21
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	7	0.21
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	17	0.21
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	20	0.21
(1,3798)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	6	0.21
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	20	0.21
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	11	0.21
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	12	0.21
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	4	0.21
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	6	0.21
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	20	0.21
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	9	0.21
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	7	0.21
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	12	0.21
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	20	0.21
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	3	0.21
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	7	0.21
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	20	0.21
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	2	0.21
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	3	0.21
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	4	0.21
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	7	0.21
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	17	0.21
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	3	0.21
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	14	0.21
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	19	0.21
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	14	0.21
(1,2885)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	2	0.21
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	2	0.21
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	10	0.21
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	8	0.21
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	15	0.21
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	8	0.21
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	12	0.21
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	11	0.21
(1,2795)	1:994:A:LYS:HB2	1:994:A:LYS:HD3	20	0.21
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	11	0.21
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	18	0.21
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	8	0.21
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	7	0.21
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	17	0.21
(1,2616)	1:987:A:MET:H	1:987:A:MET:HG2	16	0.21
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	19	0.21
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	4	0.21
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	10	0.21
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	5	0.21
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	12	0.21
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	16	0.21
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	17	0.21
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	18	0.21
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	1	0.21
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	11	0.21
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	13	0.21
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	14	0.21
(1,2278)	1:970:A:LEU:HD11	1:970:A:LEU:HA	14	0.21
(1,2278)	1:970:A:LEU:HD12	1:970:A:LEU:HA	14	0.21
(1,2278)	1:970:A:LEU:HD13	1:970:A:LEU:HA	14	0.21
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	15	0.21
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	15	0.21
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	15	0.21
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	18	0.21
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	3	0.21
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	4	0.21
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	8	0.21
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	13	0.21
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	2	0.21
(1,2202)	1:967:A:TRP:HB2	1:968:A:TRP:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	10	0.21
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	15	0.21
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	6	0.21
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	15	0.21
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	15	0.21
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	15	0.21
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	6	0.21
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	11	0.21
(1,2019)	1:973:A:VAL:H	2:701:B:MET:HE1	16	0.21
(1,2019)	1:973:A:VAL:H	2:701:B:MET:HE2	16	0.21
(1,2019)	1:973:A:VAL:H	2:701:B:MET:HE3	16	0.21
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	19	0.21
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	16	0.21
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	9	0.21
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	10	0.21
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	8	0.21
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	9	0.21
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	14	0.21
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	16	0.21
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	7	0.21
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	18	0.21
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	3	0.21
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	13	0.21
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	14	0.21
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	9	0.21
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	8	0.21
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	9	0.21
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	5	0.21
(1,1776)	2:738:B:LYS:HE3	2:738:B:LYS:HG2	10	0.21
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	7	0.21
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	7	0.21
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	17	0.21
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	20	0.21
(1,1715)	2:734:B:ARG:HD3	2:734:B:ARG:HB2	6	0.21
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	20	0.21
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	11	0.21
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	12	0.21
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	4	0.21
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	6	0.21
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	20	0.21
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	9	0.21
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	12	0.21
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	20	0.21
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	3	0.21
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	7	0.21
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	20	0.21
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	2	0.21
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	3	0.21
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	4	0.21
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	7	0.21
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	17	0.21
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	3	0.21
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	14	0.21
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	18	0.21
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	19	0.21
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	14	0.21
(1,802)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	2	0.21
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	2	0.21
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	10	0.21
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	8	0.21
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	15	0.21
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	8	0.21
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	12	0.21
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	11	0.21
(1,712)	1:994:A:LYS:HB2	1:994:A:LYS:HD3	20	0.21
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	11	0.21
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	18	0.21
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	8	0.21
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	7	0.21
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	17	0.21
(1,533)	1:987:A:MET:H	1:987:A:MET:HG2	16	0.21
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	19	0.21
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	4	0.21
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	10	0.21
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	5	0.21
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	12	0.21
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	16	0.21
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	17	0.21
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	18	0.21
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	1	0.21
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	11	0.21
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	13	0.21
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:970:A:LEU:HD11	1:970:A:LEU:HA	14	0.21
(1,195)	1:970:A:LEU:HD12	1:970:A:LEU:HA	14	0.21
(1,195)	1:970:A:LEU:HD13	1:970:A:LEU:HA	14	0.21
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	15	0.21
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	15	0.21
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	15	0.21
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	18	0.21
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	3	0.21
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	4	0.21
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	8	0.21
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	13	0.21
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	2	0.21
(1,119)	1:967:A:TRP:HB2	1:968:A:TRP:H	5	0.21
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	10	0.21
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	15	0.21
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	6	0.21
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	2	0.2
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	4	0.2
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	4	0.2
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	7	0.2
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	10	0.2
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	16	0.2
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	3	0.2
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	14	0.2
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	10	0.2
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	3	0.2
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	9	0.2
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	17	0.2
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	8	0.2
(1,3963)	2:746:B:LEU:HB2	2:747:B:TYR:H	16	0.2
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	11	0.2
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	17	0.2
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	17	0.2
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	10	0.2
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	18	0.2
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	18	0.2
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	18	0.2
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	3	0.2
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	10	0.2
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	14	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	1	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	3	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	5	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	6	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	8	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	10	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	13	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	14	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	15	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	18	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	19	0.2
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	20	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	5	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	7	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	10	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	14	0.2
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	15	0.2
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	17	0.2
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	2	0.2
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	4	0.2
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	5	0.2
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	19	0.2
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	6	0.2
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	13	0.2
(1,3303)	2:708:B:GLY:H	2:710:B:ALA:H	4	0.2
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	1	0.2
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	5	0.2
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	16	0.2
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	7	0.2
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	19	0.2
(1,2952)	2:693:B:ILE:H	2:693:B:ILE:HG12	11	0.2
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	9	0.2
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	13	0.2
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	15	0.2
(1,2932)	2:692:B:ASP:HB3	2:693:B:ILE:H	8	0.2
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	3	0.2
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	18	0.2
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	1	0.2
(1,2838)	1:997:A:ARG:H	1:997:A:ARG:HG3	19	0.2
(1,2823)	1:995:A:ARG:H	1:996:A:ASN:H	11	0.2
(1,2820)	1:995:A:ARG:HB3	1:996:A:ASN:H	18	0.2
(1,2801)	1:994:A:LYS:HB2	1:995:A:ARG:H	17	0.2
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	1	0.2
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	5	0.2
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	13	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	2	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	8	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	10	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	15	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	16	0.2
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	17	0.2
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	10	0.2
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	11	0.2
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	12	0.2
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	15	0.2
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	16	0.2
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	11	0.2
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	13	0.2
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	17	0.2
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	14	0.2
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	7	0.2
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	14	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	6	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	11	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	12	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	17	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	19	0.2
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	20	0.2
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	1	0.2
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	7	0.2
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	12	0.2
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	8	0.2
(1,2474)	1:982:A:ILE:H	1:983:A:LEU:HB3	19	0.2
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	14	0.2
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	11	0.2
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	12	0.2
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	9	0.2
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	16	0.2
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	9	0.2
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	6	0.2
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	6	0.2
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	6	0.2
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	20	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	12	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	15	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	16	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	17	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	18	0.2
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	19	0.2
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	5	0.2
(1,2196)	1:967:A:TRP:H	1:968:A:TRP:HA	2	0.2
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	2	0.2
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	4	0.2
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	4	0.2
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	7	0.2
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	10	0.2
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	16	0.2
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	3	0.2
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	14	0.2
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	10	0.2
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	3	0.2
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	9	0.2
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	17	0.2
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	8	0.2
(1,1880)	2:746:B:LEU:HB2	2:747:B:TYR:H	16	0.2
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	11	0.2
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	17	0.2
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	17	0.2
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	10	0.2
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	18	0.2
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	18	0.2
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	18	0.2
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	3	0.2
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	10	0.2
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	14	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	1	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	2	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	3	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	5	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	6	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	8	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	10	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	13	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	14	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	18	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	19	0.2
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	20	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	5	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	7	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	10	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	14	0.2
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	15	0.2
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	17	0.2
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	2	0.2
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	4	0.2
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	5	0.2
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	19	0.2
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	6	0.2
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	13	0.2
(1,1220)	2:708:B:GLY:H	2:710:B:ALA:H	4	0.2
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	1	0.2
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	5	0.2
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	16	0.2
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	7	0.2
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	19	0.2
(1,869)	2:693:B:ILE:H	2:693:B:ILE:HG12	11	0.2
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	9	0.2
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	13	0.2
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	15	0.2
(1,849)	2:692:B:ASP:HB3	2:693:B:ILE:H	8	0.2
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	3	0.2
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	18	0.2
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	1	0.2
(1,755)	1:997:A:ARG:H	1:997:A:ARG:HG3	19	0.2
(1,740)	1:995:A:ARG:H	1:996:A:ASN:H	11	0.2
(1,737)	1:995:A:ARG:HB3	1:996:A:ASN:H	18	0.2
(1,718)	1:994:A:LYS:HB2	1:995:A:ARG:H	17	0.2
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	20	0.2
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	1	0.2
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	5	0.2
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	13	0.2
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	2	0.2
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	8	0.2
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	10	0.2
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	15	0.2
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	17	0.2
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	10	0.2
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	11	0.2
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	12	0.2
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	15	0.2
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	16	0.2
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	11	0.2
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	13	0.2
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	17	0.2
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	14	0.2
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	7	0.2
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	14	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	6	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	11	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	12	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	17	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	19	0.2
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	20	0.2
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	1	0.2
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	7	0.2
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	12	0.2
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	8	0.2
(1,391)	1:982:A:ILE:H	1:983:A:LEU:HB3	19	0.2
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	14	0.2
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	11	0.2
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	12	0.2
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	9	0.2
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	16	0.2
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	9	0.2
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	6	0.2
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	6	0.2
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	6	0.2
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	20	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	11	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	12	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	15	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	16	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	17	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	18	0.2
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	19	0.2
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	5	0.2
(1,113)	1:967:A:TRP:H	1:968:A:TRP:HA	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	16	0.19
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	16	0.19
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	16	0.19
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	5	0.19
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	6	0.19
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	19	0.19
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	20	0.19
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	11	0.19
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	11	0.19
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	11	0.19
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	3	0.19
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	19	0.19
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	1	0.19
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	5	0.19
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	9	0.19
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	2	0.19
(1,4138)	1:980:A:LEU:HA	2:708:B:GLY:H	16	0.19
(1,4131)	1:979:A:LEU:H	2:707:B:ILE:HB	12	0.19
(1,4121)	1:976:A:GLY:H	2:707:B:ILE:HB	17	0.19
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	2	0.19
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	20	0.19
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	6	0.19
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	15	0.19
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	2	0.19
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	4	0.19
(1,3913)	2:743:B:ASN:H	2:743:B:ASN:HD22	6	0.19
(1,3902)	2:742:B:ALA:HA	2:743:B:ASN:H	2	0.19
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	4	0.19
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	3	0.19
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	4	0.19
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	8	0.19
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	20	0.19
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	9	0.19
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	15	0.19
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	2	0.19
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	11	0.19
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	12	0.19
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	11	0.19
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	9	0.19
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	17	0.19
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	2	0.19
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	18	0.19
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	4	0.19
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	4	0.19
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	8	0.19
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	10	0.19
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	11	0.19
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	20	0.19
(1,3508)	2:718:B:LEU:HD21	2:721:B:ILE:HB	7	0.19
(1,3508)	2:718:B:LEU:HD22	2:721:B:ILE:HB	7	0.19
(1,3508)	2:718:B:LEU:HD23	2:721:B:ILE:HB	7	0.19
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	1	0.19
(1,3454)	2:716:B:LYS:HE3	2:719:B:ILE:HG12	7	0.19
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	19	0.19
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	6	0.19
(1,2952)	2:693:B:ILE:H	2:693:B:ILE:HG12	1	0.19
(1,2926)	2:691:B:PRO:HB3	2:692:B:ASP:H	9	0.19
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	2	0.19
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	19	0.19
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	20	0.19
(1,2896)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	2	0.19
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	5	0.19
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	15	0.19
(1,2881)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	14	0.19
(1,2875)	1:1002:A:GLU:H	1:1002:A:GLU:HG3	8	0.19
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	17	0.19
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	19	0.19
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	17	0.19
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	14	0.19
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	1	0.19
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	5	0.19
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	6	0.19
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	7	0.19
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	8	0.19
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	20	0.19
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	16	0.19
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	8	0.19
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	11	0.19
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	1	0.19
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	3	0.19
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	2	0.19
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	6	0.19
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	2	0.19
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	6	0.19
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	12	0.19
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	20	0.19
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	7	0.19
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	9	0.19
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	2	0.19
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	10	0.19
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	19	0.19
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	8	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	1	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	9	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	11	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	13	0.19
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	16	0.19
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	1	0.19
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	5	0.19
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	7	0.19
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	10	0.19
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	20	0.19
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	14	0.19
(1,2107)	1:963:A:ALA:H	1:964:A:ILE:H	13	0.19
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	18	0.19
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	16	0.19
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	16	0.19
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	16	0.19
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	5	0.19
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	6	0.19
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	19	0.19
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	20	0.19
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	11	0.19
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	11	0.19
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	11	0.19
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	3	0.19
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	19	0.19
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	1	0.19
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	5	0.19
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	9	0.19
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	2	0.19
(1,2055)	1:980:A:LEU:HA	2:708:B:GLY:H	16	0.19
(1,2048)	1:979:A:LEU:H	2:707:B:ILE:HB	12	0.19
(1,2038)	1:976:A:GLY:H	2:707:B:ILE:HB	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	2	0.19
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	20	0.19
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	6	0.19
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	15	0.19
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	2	0.19
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	4	0.19
(1,1830)	2:743:B:ASN:H	2:743:B:ASN:HD22	6	0.19
(1,1819)	2:742:B:ALA:HA	2:743:B:ASN:H	2	0.19
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	4	0.19
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	3	0.19
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	4	0.19
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	8	0.19
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	20	0.19
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	9	0.19
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	15	0.19
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	2	0.19
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	11	0.19
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	12	0.19
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	11	0.19
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	9	0.19
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	17	0.19
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	2	0.19
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	11	0.19
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	18	0.19
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	4	0.19
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	4	0.19
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	8	0.19
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	10	0.19
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	11	0.19
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	20	0.19
(1,1425)	2:718:B:LEU:HD21	2:721:B:ILE:HB	7	0.19
(1,1425)	2:718:B:LEU:HD22	2:721:B:ILE:HB	7	0.19
(1,1425)	2:718:B:LEU:HD23	2:721:B:ILE:HB	7	0.19
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	1	0.19
(1,1371)	2:716:B:LYS:HE3	2:719:B:ILE:HG12	7	0.19
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	19	0.19
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	6	0.19
(1,869)	2:693:B:ILE:H	2:693:B:ILE:HG12	1	0.19
(1,843)	2:691:B:PRO:HB3	2:692:B:ASP:H	9	0.19
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	2	0.19
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	19	0.19
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	2	0.19
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	5	0.19
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	15	0.19
(1,798)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	14	0.19
(1,792)	1:1002:A:GLU:H	1:1002:A:GLU:HG3	8	0.19
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	17	0.19
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	19	0.19
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	17	0.19
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	14	0.19
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	1	0.19
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	5	0.19
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	6	0.19
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	7	0.19
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	8	0.19
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	20	0.19
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	16	0.19
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	8	0.19
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	11	0.19
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	1	0.19
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	3	0.19
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	2	0.19
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	6	0.19
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	14	0.19
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	2	0.19
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	6	0.19
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	12	0.19
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	20	0.19
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	7	0.19
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	9	0.19
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	2	0.19
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	10	0.19
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	19	0.19
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	8	0.19
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	1	0.19
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	9	0.19
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	11	0.19
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	13	0.19
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	16	0.19
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	1	0.19
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	5	0.19
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	7	0.19
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	20	0.19
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	14	0.19
(1,24)	1:963:A:ALA:H	1:964:A:ILE:H	13	0.19
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	18	0.19
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	9	0.18
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	14	0.18
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	9	0.18
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	19	0.18
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	20	0.18
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	4	0.18
(1,4130)	1:979:A:LEU:H	2:704:B:ILE:HB	18	0.18
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	9	0.18
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	18	0.18
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	6	0.18
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	1	0.18
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	3	0.18
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	16	0.18
(1,3913)	2:743:B:ASN:H	2:743:B:ASN:HD22	16	0.18
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	2	0.18
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	12	0.18
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	16	0.18
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	7	0.18
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	14	0.18
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	4	0.18
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	4	0.18
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	16	0.18
(1,3870)	2:738:B:LYS:HA	2:740:B:ASP:H	7	0.18
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	8	0.18
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	10	0.18
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	12	0.18
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	11	0.18
(1,3852)	2:738:B:LYS:H	2:738:B:LYS:HG3	15	0.18
(1,3741)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	9	0.18
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	17	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	1	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	11	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	13	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	15	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	16	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	17	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	19	0.18
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	18	0.18
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	19	0.18
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	20	0.18
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	20	0.18
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	1	0.18
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	4	0.18
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	7	0.18
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	20	0.18
(1,2924)	2:691:B:PRO:HD3	2:692:B:ASP:H	9	0.18
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	1	0.18
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	6	0.18
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	11	0.18
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	4	0.18
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	1	0.18
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	16	0.18
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	3	0.18
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	5	0.18
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	18	0.18
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	12	0.18
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	16	0.18
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	4	0.18
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	14	0.18
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	17	0.18
(1,2543)	1:984:A:VAL:HA	1:988:A:TRP:HB3	3	0.18
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	12	0.18
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	8	0.18
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	18	0.18
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	8	0.18
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	18	0.18
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	12	0.18
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	14	0.18
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	5	0.18
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	6	0.18
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	13	0.18
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	19	0.18
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	3	0.18
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	4	0.18
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	5	0.18
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	12	0.18
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	19	0.18
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	3	0.18
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	13	0.18
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	15	0.18
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	1	0.18
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	18	0.18
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	19	0.18
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	3	0.18
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	6	0.18
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	6	0.18
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	9	0.18
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	5	0.18
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	3	0.18
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	9	0.18
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	14	0.18
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	9	0.18
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	19	0.18
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	20	0.18
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	4	0.18
(1,2047)	1:979:A:LEU:H	2:704:B:ILE:HB	18	0.18
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	9	0.18
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	18	0.18
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	6	0.18
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	1	0.18
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	3	0.18
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	16	0.18
(1,1830)	2:743:B:ASN:H	2:743:B:ASN:HD22	16	0.18
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	2	0.18
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	12	0.18
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	16	0.18
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	7	0.18
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	14	0.18
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	4	0.18
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	4	0.18
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	16	0.18
(1,1787)	2:738:B:LYS:HA	2:740:B:ASP:H	7	0.18
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	8	0.18
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	10	0.18
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	12	0.18
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	11	0.18
(1,1769)	2:738:B:LYS:H	2:738:B:LYS:HG3	15	0.18
(1,1658)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	9	0.18
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	17	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	11	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	13	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	15	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	16	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	17	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	19	0.18
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	20	0.18
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	18	0.18
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	19	0.18
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	20	0.18
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	20	0.18
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	1	0.18
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	4	0.18
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	7	0.18
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	20	0.18
(1,841)	2:691:B:PRO:HD3	2:692:B:ASP:H	9	0.18
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	1	0.18
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	6	0.18
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	11	0.18
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	4	0.18
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	1	0.18
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	16	0.18
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	3	0.18
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	5	0.18
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	18	0.18
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	12	0.18
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	16	0.18
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	4	0.18
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	14	0.18
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	17	0.18
(1,460)	1:984:A:VAL:HA	1:988:A:TRP:HB3	3	0.18
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	12	0.18
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	8	0.18
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	18	0.18
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	8	0.18
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	18	0.18
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	12	0.18
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	14	0.18
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	5	0.18
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	6	0.18
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	13	0.18
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	3	0.18
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	4	0.18
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	5	0.18
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	12	0.18
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	19	0.18
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	3	0.18
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	6	0.18
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	13	0.18
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	15	0.18
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	1	0.18
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	18	0.18
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	19	0.18
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	3	0.18
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	6	0.18
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	6	0.18
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	9	0.18
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	5	0.18
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	3	0.18
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	17	0.17
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	17	0.17
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	10	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	13	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	13	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	13	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	16	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	16	0.17
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	16	0.17
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	11	0.17
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	1	0.17
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	10	0.17
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	7	0.17
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	8	0.17
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	20	0.17
(1,3963)	2:746:B:LEU:HB2	2:747:B:TYR:H	15	0.17
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	7	0.17
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	15	0.17
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	18	0.17
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	19	0.17
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	3	0.17
(1,3909)	2:743:B:ASN:HB2	2:743:B:ASN:H	15	0.17
(1,3904)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	5	0.17
(1,3904)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3904)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	5	0.17
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	20	0.17
(1,3882)	2:739:B:TRP:HB2	2:740:B:ASP:H	16	0.17
(1,3857)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	12	0.17
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	6	0.17
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	5	0.17
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	4	0.17
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	9	0.17
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	16	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	3	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	5	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	8	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	9	0.17
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	12	0.17
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	2	0.17
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	18	0.17
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	1	0.17
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	2	0.17
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	6	0.17
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	9	0.17
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	9	0.17
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	4	0.17
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	13	0.17
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	10	0.17
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	5	0.17
(1,2878)	1:1002:A:GLU:HA	1:1003:A:ASP:H	14	0.17
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	14	0.17
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	8	0.17
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	18	0.17
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	3	0.17
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	10	0.17
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	4	0.17
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	9	0.17
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	14	0.17
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	2	0.17
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	5	0.17
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	14	0.17
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	1	0.17
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	4	0.17
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	7	0.17
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	18	0.17
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	13	0.17
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	8	0.17
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	10	0.17
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	15	0.17
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	8	0.17
(1,2570)	1:985:A:LEU:H	1:987:A:MET:HG2	16	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	6	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	7	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	9	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	19	0.17
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	20	0.17
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	19	0.17
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	13	0.17
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	2	0.17
(1,2476)	1:982:A:ILE:H	1:984:A:VAL:H	4	0.17
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	11	0.17
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	12	0.17
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	3	0.17
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	7	0.17
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	8	0.17
(1,2395)	1:977:A:LEU:HD11	1:977:A:LEU:HA	5	0.17
(1,2395)	1:977:A:LEU:HD12	1:977:A:LEU:HA	5	0.17
(1,2395)	1:977:A:LEU:HD13	1:977:A:LEU:HA	5	0.17
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	15	0.17
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	18	0.17
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	8	0.17
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	10	0.17
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	17	0.17
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	6	0.17
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	7	0.17
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	13	0.17
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	10	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	13	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	13	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	13	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	16	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	16	0.17
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	16	0.17
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	11	0.17
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	1	0.17
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	10	0.17
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	8	0.17
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	20	0.17
(1,1880)	2:746:B:LEU:HB2	2:747:B:TYR:H	15	0.17
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	7	0.17
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	15	0.17
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	18	0.17
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	19	0.17
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	3	0.17
(1,1826)	2:743:B:ASN:HB2	2:743:B:ASN:H	15	0.17
(1,1821)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	5	0.17
(1,1821)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	5	0.17
(1,1821)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	5	0.17
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	20	0.17
(1,1799)	2:739:B:TRP:HB2	2:740:B:ASP:H	16	0.17
(1,1774)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	12	0.17
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	6	0.17
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	5	0.17
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	4	0.17
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	9	0.17
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	16	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	3	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	5	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	8	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	9	0.17
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	12	0.17
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	2	0.17
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	18	0.17
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	1	0.17
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	2	0.17
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	6	0.17
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	9	0.17
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	9	0.17
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	4	0.17
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	13	0.17
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	10	0.17
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	5	0.17
(1,795)	1:1002:A:GLU:HA	1:1003:A:ASP:H	14	0.17
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	14	0.17
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	8	0.17
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	18	0.17
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	3	0.17
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	4	0.17
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	9	0.17
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	14	0.17
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	2	0.17
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	5	0.17
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	14	0.17
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	1	0.17
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	4	0.17
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	7	0.17
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	18	0.17
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	2	0.17
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	13	0.17
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	8	0.17
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	10	0.17
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	15	0.17
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	8	0.17
(1,487)	1:985:A:LEU:H	1:987:A:MET:HG2	16	0.17
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	6	0.17
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	7	0.17
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	9	0.17
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	19	0.17
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	20	0.17
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	19	0.17
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	13	0.17
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	2	0.17
(1,393)	1:982:A:ILE:H	1:984:A:VAL:H	4	0.17
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	11	0.17
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	12	0.17
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	3	0.17
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	7	0.17
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	8	0.17
(1,312)	1:977:A:LEU:HD11	1:977:A:LEU:HA	5	0.17
(1,312)	1:977:A:LEU:HD12	1:977:A:LEU:HA	5	0.17
(1,312)	1:977:A:LEU:HD13	1:977:A:LEU:HA	5	0.17
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	15	0.17
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	18	0.17
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	8	0.17
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	10	0.17
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	17	0.17
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	6	0.17
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	7	0.17
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	12	0.16
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	13	0.16
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	12	0.16
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	13	0.16
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	17	0.16
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	14	0.16
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	6	0.16
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	10	0.16
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	12	0.16
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	4	0.16
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	12	0.16
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	11	0.16
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	2	0.16
(1,3973)	2:747:B:TYR:HB2	2:748:B:LYS:H	16	0.16
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	1	0.16
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	19	0.16
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	6	0.16
(1,3945)	2:745:B:PRO:HA	2:746:B:LEU:H	10	0.16
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	9	0.16
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	12	0.16
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	9	0.16
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	11	0.16
(1,3893)	2:741:B:THR:HA	2:742:B:ALA:H	15	0.16
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	8	0.16
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	10	0.16
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	14	0.16
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	17	0.16
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	17	0.16
(1,3836)	2:736:B:ARG:HG2	2:739:B:TRP:H	15	0.16
(1,3801)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	3	0.16
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	16	0.16
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	5	0.16
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	3	0.16
(1,3646)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	12	0.16
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	2	0.16
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	6	0.16
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	14	0.16
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	18	0.16
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	8	0.16
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	11	0.16
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	20	0.16
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	12	0.16
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	19	0.16
(1,3508)	2:718:B:LEU:HD21	2:721:B:ILE:HB	2	0.16
(1,3508)	2:718:B:LEU:HD22	2:721:B:ILE:HB	2	0.16
(1,3508)	2:718:B:LEU:HD23	2:721:B:ILE:HB	2	0.16
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	10	0.16
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	2	0.16
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	2	0.16
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	11	0.16
(1,3318)	2:709:B:LEU:HB3	2:710:B:ALA:HA	19	0.16
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	6	0.16
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	11	0.16
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	5	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	3	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	11	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	12	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	16	0.16
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	19	0.16
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	16	0.16
(1,2845)	1:997:A:ARG:HA	1:999:A:PRO:HD2	4	0.16
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	7	0.16
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	8	0.16
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	9	0.16
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	20	0.16
(1,2843)	1:997:A:ARG:HA	1:999:A:PRO:HD3	17	0.16
(1,2836)	1:997:A:ARG:HD3	1:997:A:ARG:HA	12	0.16
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	13	0.16
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	16	0.16
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	6	0.16
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	1	0.16
(1,2801)	1:994:A:LYS:HB2	1:995:A:ARG:H	12	0.16
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	2	0.16
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	9	0.16
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	4	0.16
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	17	0.16
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	13	0.16
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	3	0.16
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	4	0.16
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	20	0.16
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	13	0.16
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	19	0.16
(1,2694)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	1	0.16
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	2	0.16
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	4	0.16
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	18	0.16
(1,2630)	1:987:A:MET:HG3	1:989:A:LYS:H	18	0.16
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	5	0.16
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	15	0.16
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	16	0.16
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	9	0.16
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	4	0.16
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	12	0.16
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	3	0.16
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	4	0.16
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	18	0.16
(1,2425)	1:979:A:LEU:HA	1:982:A:ILE:HB	16	0.16
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	1	0.16
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	2	0.16
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	4	0.16
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	10	0.16
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	15	0.16
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	2	0.16
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	6	0.16
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	16	0.16
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	17	0.16
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	17	0.16
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	12	0.16
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	14	0.16
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	18	0.16
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	5	0.16
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	17	0.16
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	4	0.16
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	11	0.16
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	17	0.16
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	7	0.16
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	3	0.16
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	4	0.16
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	5	0.16
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	8	0.16
(1,2127)	1:964:A:ILE:H	1:965:A:PRO:HB2	11	0.16
(1,2111)	1:964:A:ILE:H	1:964:A:ILE:HB	4	0.16
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	6	0.16
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	16	0.16
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	8	0.16
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	17	0.16
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	14	0.16
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	6	0.16
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	10	0.16
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	12	0.16
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	4	0.16
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	12	0.16
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	11	0.16
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	2	0.16
(1,1890)	2:747:B:TYR:HB2	2:748:B:LYS:H	16	0.16
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	1	0.16
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	19	0.16
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	6	0.16
(1,1862)	2:745:B:PRO:HA	2:746:B:LEU:H	10	0.16
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	9	0.16
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	12	0.16
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	9	0.16
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	11	0.16
(1,1810)	2:741:B:THR:HA	2:742:B:ALA:H	15	0.16
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	8	0.16
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	10	0.16
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	14	0.16
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	17	0.16
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	17	0.16
(1,1753)	2:736:B:ARG:HG2	2:739:B:TRP:H	15	0.16
(1,1718)	2:734:B:ARG:HD2	2:734:B:ARG:HB2	3	0.16
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	16	0.16
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	5	0.16
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	3	0.16
(1,1563)	2:725:B:LYS:HE3	2:725:B:LYS:HB3	12	0.16
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	2	0.16
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	6	0.16
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	14	0.16
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	18	0.16
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	8	0.16
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	11	0.16
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	20	0.16
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	7	0.16
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	12	0.16
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1425)	2:718:B:LEU:HD21	2:721:B:ILE:HB	2	0.16
(1,1425)	2:718:B:LEU:HD22	2:721:B:ILE:HB	2	0.16
(1,1425)	2:718:B:LEU:HD23	2:721:B:ILE:HB	2	0.16
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	10	0.16
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	2	0.16
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	2	0.16
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	11	0.16
(1,1235)	2:709:B:LEU:HB3	2:710:B:ALA:HA	19	0.16
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	6	0.16
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	11	0.16
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	5	0.16
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	3	0.16
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	11	0.16
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	12	0.16
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	16	0.16
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	19	0.16
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	16	0.16
(1,762)	1:997:A:ARG:HA	1:999:A:PRO:HD2	4	0.16
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	7	0.16
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	8	0.16
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	9	0.16
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	20	0.16
(1,760)	1:997:A:ARG:HA	1:999:A:PRO:HD3	17	0.16
(1,753)	1:997:A:ARG:HD3	1:997:A:ARG:HA	12	0.16
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	13	0.16
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	16	0.16
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	6	0.16
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	1	0.16
(1,718)	1:994:A:LYS:HB2	1:995:A:ARG:H	12	0.16
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	2	0.16
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	9	0.16
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	4	0.16
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	17	0.16
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	13	0.16
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	3	0.16
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	4	0.16
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	20	0.16
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	13	0.16
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	19	0.16
(1,611)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	18	0.16
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	1	0.16
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	4	0.16
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	18	0.16
(1,547)	1:987:A:MET:HG3	1:989:A:LYS:H	18	0.16
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	5	0.16
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	15	0.16
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	16	0.16
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	9	0.16
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	4	0.16
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	12	0.16
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	3	0.16
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	4	0.16
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	18	0.16
(1,342)	1:979:A:LEU:HA	1:982:A:ILE:HB	16	0.16
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	1	0.16
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	2	0.16
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	4	0.16
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	10	0.16
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	15	0.16
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	2	0.16
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	6	0.16
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	16	0.16
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	17	0.16
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	17	0.16
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	12	0.16
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	14	0.16
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	18	0.16
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	5	0.16
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	17	0.16
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	4	0.16
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	11	0.16
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	17	0.16
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	7	0.16
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	3	0.16
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	4	0.16
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	5	0.16
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	8	0.16
(1,44)	1:964:A:ILE:H	1:965:A:PRO:HB2	11	0.16
(1,28)	1:964:A:ILE:H	1:964:A:ILE:HB	4	0.16
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	6	0.16
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	7	0.16
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	16	0.16
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	1	0.15
(3,211)	1:984:A:VAL:O	1:987:A:MET:H	16	0.15
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	1	0.15
(3,52)	1:984:A:VAL:O	1:987:A:MET:H	16	0.15
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	3	0.15
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	8	0.15
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	9	0.15
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	9	0.15
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	9	0.15
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	5	0.15
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	2	0.15
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	18	0.15
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	13	0.15
(1,4132)	1:979:A:LEU:HD21	2:708:B:GLY:H	6	0.15
(1,4132)	1:979:A:LEU:HD22	2:708:B:GLY:H	6	0.15
(1,4132)	1:979:A:LEU:HD23	2:708:B:GLY:H	6	0.15
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	9	0.15
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	18	0.15
(1,4053)	2:757:B:ILE:H	2:757:B:ILE:HG13	2	0.15
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	1	0.15
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	11	0.15
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	19	0.15
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	12	0.15
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	19	0.15
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	13	0.15
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	18	0.15
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	19	0.15
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	12	0.15
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	18	0.15
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	17	0.15
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	5	0.15
(1,3904)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	9	0.15
(1,3904)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	9	0.15
(1,3904)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	9	0.15
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	3	0.15
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	15	0.15
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	17	0.15
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	1	0.15
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	4	0.15
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	13	0.15
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	20	0.15
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	10	0.15
(1,3746)	2:730:B:PHE:HE1	2:734:B:ARG:HG3	19	0.15
(1,3718)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	7	0.15
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	7	0.15
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	10	0.15
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	15	0.15
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	1	0.15
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	19	0.15
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	3	0.15
(1,3507)	2:718:B:LEU:HD11	2:721:B:ILE:HB	13	0.15
(1,3507)	2:718:B:LEU:HD12	2:721:B:ILE:HB	13	0.15
(1,3507)	2:718:B:LEU:HD13	2:721:B:ILE:HB	13	0.15
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	5	0.15
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	6	0.15
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	10	0.15
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	5	0.15
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	7	0.15
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	8	0.15
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	14	0.15
(1,3126)	2:700:B:VAL:HB	2:701:B:MET:HG2	8	0.15
(1,3059)	2:697:B:LEU:HB3	2:699:B:SER:H	5	0.15
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	10	0.15
(1,2896)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	13	0.15
(1,2881)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	13	0.15
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	7	0.15
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	17	0.15
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	3	0.15
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	7	0.15
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	12	0.15
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	16	0.15
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	12	0.15
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	20	0.15
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	17	0.15
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	6	0.15
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	12	0.15
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	3	0.15
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	12	0.15
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	14	0.15
(1,2616)	1:987:A:MET:H	1:987:A:MET:HG2	18	0.15
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	2	0.15
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	8	0.15
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2568)	1:985:A:LEU:HA	1:987:A:MET:H	18	0.15
(1,2533)	1:984:A:VAL:HA	1:987:A:MET:H	10	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	1	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	1	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	1	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	7	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	7	0.15
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	7	0.15
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	1	0.15
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	9	0.15
(1,2495)	1:983:A:LEU:HD11	1:983:A:LEU:H	1	0.15
(1,2495)	1:983:A:LEU:HD12	1:983:A:LEU:H	1	0.15
(1,2495)	1:983:A:LEU:HD13	1:983:A:LEU:H	1	0.15
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	7	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	2	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	4	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	9	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	10	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	19	0.15
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	20	0.15
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	11	0.15
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	10	0.15
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	17	0.15
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	20	0.15
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	9	0.15
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	1	0.15
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	2	0.15
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	4	0.15
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	5	0.15
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	13	0.15
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	15	0.15
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	10	0.15
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD21	11	0.15
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD22	11	0.15
(1,2273)	1:970:A:LEU:H	1:970:A:LEU:HD23	11	0.15
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	9	0.15
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	2	0.15
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	15	0.15
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	15	0.15
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	2	0.15
(1,2208)	1:967:A:TRP:H	1:970:A:LEU:H	6	0.15
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	9	0.15
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	4	0.15
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	13	0.15
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	3	0.15
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	8	0.15
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	9	0.15
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	9	0.15
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	9	0.15
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	5	0.15
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	2	0.15
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	18	0.15
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	13	0.15
(1,2049)	1:979:A:LEU:HD21	2:708:B:GLY:H	6	0.15
(1,2049)	1:979:A:LEU:HD22	2:708:B:GLY:H	6	0.15
(1,2049)	1:979:A:LEU:HD23	2:708:B:GLY:H	6	0.15
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	9	0.15
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	18	0.15
(1,1970)	2:757:B:ILE:H	2:757:B:ILE:HG13	2	0.15
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	1	0.15
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	11	0.15
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	19	0.15
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	12	0.15
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	19	0.15
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	13	0.15
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	18	0.15
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	19	0.15
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	12	0.15
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	18	0.15
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	17	0.15
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	5	0.15
(1,1821)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	9	0.15
(1,1821)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	9	0.15
(1,1821)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	9	0.15
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	3	0.15
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	15	0.15
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	17	0.15
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	1	0.15
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	4	0.15
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	13	0.15
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	20	0.15
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	5	0.15
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1663)	2:730:B:PHE:HE1	2:734:B:ARG:HG3	19	0.15
(1,1635)	2:729:B:LYS:HE3	2:729:B:LYS:HB3	7	0.15
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	7	0.15
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	10	0.15
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	15	0.15
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	1	0.15
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	19	0.15
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	3	0.15
(1,1424)	2:718:B:LEU:HD11	2:721:B:ILE:HB	13	0.15
(1,1424)	2:718:B:LEU:HD12	2:721:B:ILE:HB	13	0.15
(1,1424)	2:718:B:LEU:HD13	2:721:B:ILE:HB	13	0.15
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	5	0.15
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	6	0.15
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	10	0.15
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	5	0.15
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	7	0.15
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	8	0.15
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	14	0.15
(1,1043)	2:700:B:VAL:HB	2:701:B:MET:HG2	8	0.15
(1,976)	2:697:B:LEU:HB3	2:699:B:SER:H	5	0.15
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	10	0.15
(1,813)	1:1006:A:GLU:H	1:1006:A:GLU:HB2	13	0.15
(1,798)	1:1003:A:ASP:H	1:1003:A:ASP:HB2	13	0.15
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	7	0.15
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	17	0.15
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	3	0.15
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	7	0.15
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	12	0.15
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	16	0.15
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	12	0.15
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	20	0.15
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	17	0.15
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	6	0.15
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	12	0.15
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	3	0.15
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	12	0.15
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	14	0.15
(1,533)	1:987:A:MET:H	1:987:A:MET:HG2	18	0.15
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	2	0.15
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	8	0.15
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	10	0.15
(1,485)	1:985:A:LEU:HA	1:987:A:MET:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:984:A:VAL:HA	1:987:A:MET:H	10	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	1	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	1	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	1	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	7	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	7	0.15
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	7	0.15
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	1	0.15
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	9	0.15
(1,412)	1:983:A:LEU:HD11	1:983:A:LEU:H	1	0.15
(1,412)	1:983:A:LEU:HD12	1:983:A:LEU:H	1	0.15
(1,412)	1:983:A:LEU:HD13	1:983:A:LEU:H	1	0.15
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	7	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	2	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	4	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	9	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	10	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	19	0.15
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	20	0.15
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	11	0.15
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	10	0.15
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	17	0.15
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	20	0.15
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	9	0.15
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	1	0.15
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	2	0.15
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	4	0.15
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	5	0.15
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	13	0.15
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	15	0.15
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	10	0.15
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD21	11	0.15
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD22	11	0.15
(1,190)	1:970:A:LEU:H	1:970:A:LEU:HD23	11	0.15
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	9	0.15
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	2	0.15
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	15	0.15
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	15	0.15
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	2	0.15
(1,125)	1:967:A:TRP:H	1:970:A:LEU:H	6	0.15
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	8	0.15
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	4	0.15
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	13	0.15
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	10	0.14
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	20	0.14
(3,240)	2:700:B:VAL:O	2:704:B:ILE:H	1	0.14
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	1	0.14
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	3	0.14
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	17	0.14
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	19	0.14
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	10	0.14
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	20	0.14
(3,81)	2:700:B:VAL:O	2:704:B:ILE:H	1	0.14
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	1	0.14
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	3	0.14
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	17	0.14
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	19	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	4	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	4	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	4	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	7	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	7	0.14
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	7	0.14
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	8	0.14
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	15	0.14
(1,4155)	1:988:A:TRP:H	2:715:B:TRP:HB3	16	0.14
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	11	0.14
(1,4143)	1:984:A:VAL:H	2:712:B:LEU:HA	12	0.14
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	18	0.14
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	4	0.14
(1,4093)	1:969:A:VAL:HA	2:700:B:VAL:H	16	0.14
(1,4085)	1:968:A:TRP:HE1	2:693:B:ILE:HB	12	0.14
(1,4040)	2:756:B:ASN:H	2:756:B:ASN:HB2	12	0.14
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	5	0.14
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	5	0.14
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	12	0.14
(1,3918)	2:743:B:ASN:HA	2:744:B:ASN:H	14	0.14
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	18	0.14
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	5	0.14
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	7	0.14
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	5	0.14
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	6	0.14
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	16	0.14
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	19	0.14
(1,3860)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	2	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	1	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	3	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	4	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	8	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	9	0.14
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	16	0.14
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	7	0.14
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	15	0.14
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	7	0.14
(1,3644)	2:725:B:LYS:H	2:725:B:LYS:HG3	10	0.14
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	14	0.14
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	5	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	4	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	5	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	7	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	8	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	11	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	13	0.14
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	15	0.14
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	13	0.14
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	17	0.14
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	17	0.14
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	17	0.14
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	4	0.14
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	15	0.14
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	18	0.14
(1,3211)	2:704:B:ILE:HB	2:705:B:LEU:HB2	17	0.14
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	16	0.14
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	2	0.14
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	11	0.14
(1,2931)	2:692:B:ASP:H	2:692:B:ASP:HB3	15	0.14
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	4	0.14
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	13	0.14
(1,2886)	1:1004:A:ASP:HA	1:1005:A:GLU:H	13	0.14
(1,2886)	1:1004:A:ASP:HA	1:1005:A:GLU:H	15	0.14
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	11	0.14
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	5	0.14
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	2	0.14
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	7	0.14
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	9	0.14
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	12	0.14
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	15	0.14
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	16	0.14
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	1	0.14
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	16	0.14
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	7	0.14
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	15	0.14
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	9	0.14
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	7	0.14
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	2	0.14
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	10	0.14
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	7	0.14
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	14	0.14
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	15	0.14
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	6	0.14
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	9	0.14
(1,2570)	1:985:A:LEU:H	1:987:A:MET:HG2	18	0.14
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	6	0.14
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	16	0.14
(1,2506)	1:983:A:LEU:H	1:985:A:LEU:H	16	0.14
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	9	0.14
(1,2443)	1:980:A:LEU:HA	1:983:A:LEU:HB3	17	0.14
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	1	0.14
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	3	0.14
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	6	0.14
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	7	0.14
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	15	0.14
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	9	0.14
(1,2424)	1:979:A:LEU:HA	1:981:A:THR:H	18	0.14
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	1	0.14
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	7	0.14
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	10	0.14
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	11	0.14
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	2	0.14
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	19	0.14
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	11	0.14
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	13	0.14
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	4	0.14
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	11	0.14
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	12	0.14
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	2	0.14
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	8	0.14
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	12	0.14
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	20	0.14
(1,2201)	1:967:A:TRP:HA	1:968:A:TRP:HB3	11	0.14
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	4	0.14
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	5	0.14
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	11	0.14
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	14	0.14
(1,2129)	1:964:A:ILE:HB	1:965:A:PRO:HD2	2	0.14
(1,2129)	1:964:A:ILE:HB	1:965:A:PRO:HD2	6	0.14
(1,2097)	1:962:A:ARG:H	1:962:A:ARG:HB2	4	0.14
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	6	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	4	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	4	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	4	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	7	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	7	0.14
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	7	0.14
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	8	0.14
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	15	0.14
(1,2072)	1:988:A:TRP:H	2:715:B:TRP:HB3	16	0.14
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	11	0.14
(1,2060)	1:984:A:VAL:H	2:712:B:LEU:HA	12	0.14
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	18	0.14
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	4	0.14
(1,2010)	1:969:A:VAL:HA	2:700:B:VAL:H	16	0.14
(1,2002)	1:968:A:TRP:HE1	2:693:B:ILE:HB	12	0.14
(1,1957)	2:756:B:ASN:H	2:756:B:ASN:HB2	12	0.14
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	5	0.14
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	5	0.14
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	12	0.14
(1,1835)	2:743:B:ASN:HA	2:744:B:ASN:H	14	0.14
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	18	0.14
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	5	0.14
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	7	0.14
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	5	0.14
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	6	0.14
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	7	0.14
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	16	0.14
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1777)	2:738:B:LYS:HB3	2:738:B:LYS:HD3	2	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	1	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	3	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	4	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	8	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	9	0.14
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	16	0.14
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	7	0.14
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	15	0.14
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	7	0.14
(1,1561)	2:725:B:LYS:H	2:725:B:LYS:HG3	10	0.14
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	14	0.14
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	5	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	4	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	5	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	7	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	8	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	11	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	13	0.14
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	15	0.14
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	13	0.14
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	17	0.14
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	17	0.14
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	17	0.14
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	4	0.14
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	15	0.14
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	18	0.14
(1,1128)	2:704:B:ILE:HB	2:705:B:LEU:HB2	17	0.14
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	16	0.14
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	2	0.14
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	11	0.14
(1,848)	2:692:B:ASP:H	2:692:B:ASP:HB3	15	0.14
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	4	0.14
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	13	0.14
(1,803)	1:1004:A:ASP:HA	1:1005:A:GLU:H	13	0.14
(1,803)	1:1004:A:ASP:HA	1:1005:A:GLU:H	15	0.14
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	11	0.14
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	5	0.14
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	2	0.14
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	2	0.14
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	7	0.14
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	12	0.14
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	15	0.14
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	16	0.14
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	1	0.14
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	16	0.14
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	7	0.14
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	15	0.14
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	9	0.14
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	7	0.14
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	2	0.14
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	10	0.14
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	7	0.14
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	14	0.14
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	15	0.14
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	6	0.14
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	9	0.14
(1,487)	1:985:A:LEU:H	1:987:A:MET:HG2	18	0.14
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	6	0.14
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	16	0.14
(1,423)	1:983:A:LEU:H	1:985:A:LEU:H	16	0.14
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	9	0.14
(1,360)	1:980:A:LEU:HA	1:983:A:LEU:HB3	17	0.14
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	1	0.14
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	3	0.14
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	6	0.14
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	7	0.14
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	15	0.14
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	9	0.14
(1,341)	1:979:A:LEU:HA	1:981:A:THR:H	18	0.14
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	1	0.14
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	7	0.14
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	10	0.14
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	11	0.14
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	2	0.14
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	19	0.14
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	11	0.14
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	13	0.14
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	4	0.14
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	11	0.14
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	18	0.14
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	12	0.14
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	8	0.14
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	12	0.14
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	20	0.14
(1,118)	1:967:A:TRP:HA	1:968:A:TRP:HB3	11	0.14
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	4	0.14
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	5	0.14
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	11	0.14
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	14	0.14
(1,46)	1:964:A:ILE:HB	1:965:A:PRO:HD2	2	0.14
(1,46)	1:964:A:ILE:HB	1:965:A:PRO:HD2	6	0.14
(1,14)	1:962:A:ARG:H	1:962:A:ARG:HB2	4	0.14
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	6	0.14
(3,211)	1:984:A:VAL:O	1:987:A:MET:H	8	0.13
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	15	0.13
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	16	0.13
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	6	0.13
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	10	0.13
(3,52)	1:984:A:VAL:O	1:987:A:MET:H	8	0.13
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	15	0.13
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	16	0.13
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	6	0.13
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	10	0.13
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	12	0.13
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	12	0.13
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	12	0.13
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	12	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	2	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	2	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	2	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	6	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	6	0.13
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	6	0.13
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	4	0.13
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	10	0.13
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	17	0.13
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	8	0.13
(1,4131)	1:979:A:LEU:H	2:707:B:ILE:HB	16	0.13
(1,4121)	1:976:A:GLY:H	2:707:B:ILE:HB	11	0.13
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	16	0.13
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	5	0.13
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	13	0.13
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	17	0.13
(1,4040)	2:756:B:ASN:H	2:756:B:ASN:HB2	10	0.13
(1,4033)	2:754:B:PHE:HA	2:755:B:THR:H	1	0.13
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	7	0.13
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	8	0.13
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	13	0.13
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	16	0.13
(1,4028)	2:754:B:PHE:H	2:754:B:PHE:HB2	8	0.13
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	8	0.13
(1,4014)	2:751:B:THR:HA	2:752:B:SER:H	4	0.13
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG21	10	0.13
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG22	10	0.13
(1,4010)	2:751:B:THR:H	2:751:B:THR:HG23	10	0.13
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	3	0.13
(1,3963)	2:746:B:LEU:HB2	2:747:B:TYR:H	6	0.13
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	1	0.13
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	2	0.13
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	9	0.13
(1,3903)	2:742:B:ALA:HB1	2:743:B:ASN:H	15	0.13
(1,3903)	2:742:B:ALA:HB2	2:743:B:ASN:H	15	0.13
(1,3903)	2:742:B:ALA:HB3	2:743:B:ASN:H	15	0.13
(1,3894)	2:741:B:THR:HB	2:742:B:ALA:H	19	0.13
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	2	0.13
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	3	0.13
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	17	0.13
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	9	0.13
(1,3863)	2:738:B:LYS:HB3	2:739:B:TRP:H	3	0.13
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	6	0.13
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	13	0.13
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	18	0.13
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	20	0.13
(1,3668)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	6	0.13
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	1	0.13
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	5	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	1	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	6	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	9	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	13	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	15	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	17	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	18	0.13
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	1	0.13
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	2	0.13
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	14	0.13
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	18	0.13
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	20	0.13
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	4	0.13
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	5	0.13
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	15	0.13
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	18	0.13
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	19	0.13
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	19	0.13
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	19	0.13
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	15	0.13
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	7	0.13
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	16	0.13
(1,3356)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	5	0.13
(1,3356)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	15	0.13
(1,3321)	2:709:B:LEU:HA	2:712:B:LEU:HB2	4	0.13
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	3	0.13
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	7	0.13
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	9	0.13
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	12	0.13
(1,3148)	2:701:B:MET:HG3	2:704:B:ILE:HG13	6	0.13
(1,3048)	2:697:B:LEU:H	2:697:B:LEU:HB3	7	0.13
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	3	0.13
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	10	0.13
(1,2947)	2:692:B:ASP:H	2:696:B:VAL:H	17	0.13
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	5	0.13
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	12	0.13
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	16	0.13
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	14	0.13
(1,2904)	2:689:B:LYS:H	2:689:B:LYS:HD2	8	0.13
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	9	0.13
(1,2884)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	17	0.13
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	9	0.13
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	18	0.13
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	2	0.13
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	15	0.13
(1,2823)	1:995:A:ARG:H	1:996:A:ASN:H	6	0.13
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	10	0.13
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	4	0.13
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2801)	1:994:A:LYS:HB2	1:995:A:ARG:H	9	0.13
(1,2784)	1:993:A:PHE:HA	1:996:A:ASN:H	9	0.13
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	19	0.13
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	10	0.13
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	11	0.13
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	9	0.13
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	15	0.13
(1,2728)	1:990:A:VAL:HB	1:993:A:PHE:H	17	0.13
(1,2721)	1:990:A:VAL:H	1:992:A:PHE:H	9	0.13
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	5	0.13
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	10	0.13
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	19	0.13
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	7	0.13
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	13	0.13
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	20	0.13
(1,2615)	1:987:A:MET:H	1:987:A:MET:HG3	1	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	4	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	4	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	4	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	17	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	17	0.13
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	17	0.13
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	13	0.13
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	2	0.13
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	10	0.13
(1,2509)	1:983:A:LEU:HA	1:985:A:LEU:H	11	0.13
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	5	0.13
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	5	0.13
(1,2439)	1:980:A:LEU:HB3	1:981:A:THR:HA	13	0.13
(1,2425)	1:979:A:LEU:HA	1:982:A:ILE:HB	14	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	2	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	8	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	9	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	14	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	19	0.13
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	20	0.13
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	17	0.13
(1,2396)	1:977:A:LEU:HB2	1:978:A:LEU:H	5	0.13
(1,2372)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	16	0.13
(1,2356)	1:974:A:LEU:H	1:975:A:GLY:HA2	5	0.13
(1,2326)	1:972:A:GLY:H	1:976:A:GLY:H	8	0.13
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	3	0.13
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	6	0.13
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	7	0.13
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	19	0.13
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	2	0.13
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	20	0.13
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	9	0.13
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	11	0.13
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	13	0.13
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	9	0.13
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	12	0.13
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	2	0.13
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	5	0.13
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	12	0.13
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	12	0.13
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	12	0.13
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	12	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	2	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	2	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	2	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	6	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	6	0.13
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	6	0.13
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	4	0.13
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	10	0.13
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	17	0.13
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	8	0.13
(1,2048)	1:979:A:LEU:H	2:707:B:ILE:HB	16	0.13
(1,2038)	1:976:A:GLY:H	2:707:B:ILE:HB	11	0.13
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	16	0.13
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	5	0.13
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	13	0.13
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	15	0.13
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	17	0.13
(1,1957)	2:756:B:ASN:H	2:756:B:ASN:HB2	10	0.13
(1,1950)	2:754:B:PHE:HA	2:755:B:THR:H	1	0.13
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	7	0.13
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	8	0.13
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	13	0.13
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	16	0.13
(1,1945)	2:754:B:PHE:H	2:754:B:PHE:HB2	8	0.13
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	2:751:B:THR:HA	2:752:B:SER:H	4	0.13
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG21	10	0.13
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG22	10	0.13
(1,1927)	2:751:B:THR:H	2:751:B:THR:HG23	10	0.13
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	3	0.13
(1,1880)	2:746:B:LEU:HB2	2:747:B:TYR:H	6	0.13
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	1	0.13
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	2	0.13
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	9	0.13
(1,1820)	2:742:B:ALA:HB1	2:743:B:ASN:H	15	0.13
(1,1820)	2:742:B:ALA:HB2	2:743:B:ASN:H	15	0.13
(1,1820)	2:742:B:ALA:HB3	2:743:B:ASN:H	15	0.13
(1,1811)	2:741:B:THR:HB	2:742:B:ALA:H	19	0.13
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	2	0.13
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	3	0.13
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	17	0.13
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	9	0.13
(1,1780)	2:738:B:LYS:HB3	2:739:B:TRP:H	3	0.13
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	6	0.13
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	13	0.13
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	18	0.13
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	20	0.13
(1,1585)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	6	0.13
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	1	0.13
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	5	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	1	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	6	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	9	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	13	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	15	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	17	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	18	0.13
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	19	0.13
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	1	0.13
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	2	0.13
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	14	0.13
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	18	0.13
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	20	0.13
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	4	0.13
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	5	0.13
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	15	0.13
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	19	0.13
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	19	0.13
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	19	0.13
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	15	0.13
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	7	0.13
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	16	0.13
(1,1273)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	5	0.13
(1,1273)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	15	0.13
(1,1238)	2:709:B:LEU:HA	2:712:B:LEU:HB2	4	0.13
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	3	0.13
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	7	0.13
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	9	0.13
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	12	0.13
(1,1065)	2:701:B:MET:HG3	2:704:B:ILE:HG13	6	0.13
(1,965)	2:697:B:LEU:H	2:697:B:LEU:HB3	7	0.13
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	3	0.13
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	10	0.13
(1,864)	2:692:B:ASP:H	2:696:B:VAL:H	17	0.13
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	5	0.13
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	12	0.13
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	16	0.13
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	14	0.13
(1,821)	2:689:B:LYS:H	2:689:B:LYS:HD2	8	0.13
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	9	0.13
(1,801)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	17	0.13
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	9	0.13
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	18	0.13
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	2	0.13
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	15	0.13
(1,740)	1:995:A:ARG:H	1:996:A:ASN:H	6	0.13
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	10	0.13
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	4	0.13
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	5	0.13
(1,718)	1:994:A:LYS:HB2	1:995:A:ARG:H	9	0.13
(1,701)	1:993:A:PHE:HA	1:996:A:ASN:H	9	0.13
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	19	0.13
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	10	0.13
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	11	0.13
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	9	0.13
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	15	0.13
(1,645)	1:990:A:VAL:HB	1:993:A:PHE:H	17	0.13
(1,638)	1:990:A:VAL:H	1:992:A:PHE:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	5	0.13
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	10	0.13
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	19	0.13
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	7	0.13
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	13	0.13
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	20	0.13
(1,532)	1:987:A:MET:H	1:987:A:MET:HG3	1	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	4	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	4	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	4	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	17	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	17	0.13
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	17	0.13
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	13	0.13
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	2	0.13
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	10	0.13
(1,426)	1:983:A:LEU:HA	1:985:A:LEU:H	11	0.13
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	5	0.13
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	5	0.13
(1,356)	1:980:A:LEU:HB3	1:981:A:THR:HA	13	0.13
(1,342)	1:979:A:LEU:HA	1:982:A:ILE:HB	14	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	2	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	8	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	9	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	14	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	19	0.13
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	20	0.13
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	17	0.13
(1,313)	1:977:A:LEU:HB2	1:978:A:LEU:H	5	0.13
(1,289)	1:975:A:GLY:HA3	1:978:A:LEU:HB3	16	0.13
(1,273)	1:974:A:LEU:H	1:975:A:GLY:HA2	5	0.13
(1,243)	1:972:A:GLY:H	1:976:A:GLY:H	8	0.13
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	19	0.13
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	3	0.13
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	6	0.13
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	7	0.13
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	19	0.13
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	2	0.13
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	20	0.13
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	9	0.13
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	11	0.13
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	9	0.13
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	12	0.13
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	2	0.13
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	5	0.13
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	4	0.12
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	11	0.12
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	13	0.12
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	19	0.12
(3,240)	2:700:B:VAL:O	2:704:B:ILE:H	20	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	5	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	7	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	8	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	12	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	18	0.12
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	20	0.12
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	5	0.12
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	4	0.12
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	11	0.12
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	13	0.12
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	19	0.12
(3,81)	2:700:B:VAL:O	2:704:B:ILE:H	20	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	5	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	7	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	8	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	12	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	18	0.12
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	20	0.12
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	5	0.12
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	11	0.12
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	11	0.12
(1,4163)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	11	0.12
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	19	0.12
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	19	0.12
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	19	0.12
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	1	0.12
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	6	0.12
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	11	0.12
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	20	0.12
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	1	0.12
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	2	0.12
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	15	0.12
(1,4118)	1:976:A:GLY:H	2:704:B:ILE:HB	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	11	0.12
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	8	0.12
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	12	0.12
(1,4093)	1:969:A:VAL:HA	2:700:B:VAL:H	7	0.12
(1,4073)	2:759:B:TYR:HA	2:760:B:ARG:H	9	0.12
(1,4051)	2:757:B:ILE:H	2:757:B:ILE:HG12	13	0.12
(1,4038)	2:755:B:THR:H	2:756:B:ASN:H	11	0.12
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	14	0.12
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	1	0.12
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	2	0.12
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	6	0.12
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	9	0.12
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	7	0.12
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	9	0.12
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	17	0.12
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	4	0.12
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	10	0.12
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	14	0.12
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	16	0.12
(1,3944)	2:745:B:PRO:HD2	2:746:B:LEU:H	16	0.12
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	1	0.12
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	4	0.12
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	11	0.12
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	19	0.12
(1,3904)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	16	0.12
(1,3904)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	16	0.12
(1,3904)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	16	0.12
(1,3894)	2:741:B:THR:HB	2:742:B:ALA:H	6	0.12
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	5	0.12
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	6	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	6	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	11	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	12	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	13	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	14	0.12
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	18	0.12
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	16	0.12
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	18	0.12
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	11	0.12
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	14	0.12
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	19	0.12
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3744)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	11	0.12
(1,3741)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	7	0.12
(1,3708)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	7	0.12
(1,3708)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	7	0.12
(1,3708)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	7	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	1	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	3	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	4	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	8	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	9	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	10	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	11	0.12
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	18	0.12
(1,3666)	2:725:B:LYS:HA	2:729:B:LYS:HE3	4	0.12
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	3	0.12
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	6	0.12
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	14	0.12
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	20	0.12
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	3	0.12
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	6	0.12
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	10	0.12
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	12	0.12
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	16	0.12
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	8	0.12
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	11	0.12
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	20	0.12
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	1	0.12
(1,3319)	2:709:B:LEU:H	2:711:B:ALA:H	14	0.12
(1,3318)	2:709:B:LEU:HB3	2:710:B:ALA:HA	20	0.12
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	11	0.12
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	20	0.12
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	5	0.12
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	17	0.12
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	12	0.12
(1,2953)	2:693:B:ILE:H	2:693:B:ILE:HB	16	0.12
(1,2947)	2:692:B:ASP:H	2:696:B:VAL:H	1	0.12
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	9	0.12
(1,2931)	2:692:B:ASP:H	2:692:B:ASP:HB3	14	0.12
(1,2931)	2:692:B:ASP:H	2:692:B:ASP:HB3	16	0.12
(1,2903)	2:689:B:LYS:H	2:689:B:LYS:HB2	7	0.12
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	1	0.12
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	2	0.12
(1,2885)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	13	0.12
(1,2861)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	15	0.12
(1,2857)	1:999:A:PRO:HB2	1:1000:A:LEU:H	6	0.12
(1,2843)	1:997:A:ARG:HA	1:999:A:PRO:HD3	13	0.12
(1,2834)	1:996:A:ASN:H	1:997:A:ARG:H	17	0.12
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	12	0.12
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	13	0.12
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	2	0.12
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	14	0.12
(1,2807)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	14	0.12
(1,2801)	1:994:A:LYS:HB2	1:995:A:ARG:H	11	0.12
(1,2790)	1:994:A:LYS:HE3	1:994:A:LYS:HG3	19	0.12
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	4	0.12
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	10	0.12
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	16	0.12
(1,2780)	1:993:A:PHE:H	1:995:A:ARG:H	12	0.12
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	7	0.12
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	8	0.12
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	13	0.12
(1,2721)	1:990:A:VAL:H	1:992:A:PHE:H	1	0.12
(1,2694)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	11	0.12
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	2	0.12
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	6	0.12
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	13	0.12
(1,2534)	1:984:A:VAL:H	1:987:A:MET:H	1	0.12
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	20	0.12
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	20	0.12
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	20	0.12
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	14	0.12
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	9	0.12
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	20	0.12
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	13	0.12
(1,2414)	1:978:A:LEU:HA	1:981:A:THR:H	17	0.12
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	8	0.12
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	9	0.12
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	13	0.12
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	5	0.12
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	10	0.12
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	3	0.12
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	5	0.12
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2272)	1:970:A:LEU:H	1:970:A:LEU:HB3	20	0.12
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	12	0.12
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	13	0.12
(1,2266)	1:969:A:VAL:H	1:972:A:GLY:HA3	14	0.12
(1,2258)	1:969:A:VAL:H	1:970:A:LEU:HB3	7	0.12
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	3	0.12
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	7	0.12
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	8	0.12
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	1	0.12
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	4	0.12
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	10	0.12
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	15	0.12
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	10	0.12
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	16	0.12
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	3	0.12
(1,2146)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	2	0.12
(1,2146)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	6	0.12
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	15	0.12
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	18	0.12
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	7	0.12
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	10	0.12
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	14	0.12
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	17	0.12
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG21	11	0.12
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG22	11	0.12
(1,2080)	1:988:A:TRP:HE1	2:719:B:ILE:HG23	11	0.12
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	19	0.12
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	19	0.12
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	19	0.12
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	1	0.12
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	6	0.12
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	11	0.12
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	20	0.12
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	1	0.12
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	2	0.12
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	15	0.12
(1,2035)	1:976:A:GLY:H	2:704:B:ILE:HB	6	0.12
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	11	0.12
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	8	0.12
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	12	0.12
(1,2010)	1:969:A:VAL:HA	2:700:B:VAL:H	7	0.12
(1,1990)	2:759:B:TYR:HA	2:760:B:ARG:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	2:757:B:ILE:H	2:757:B:ILE:HG12	13	0.12
(1,1955)	2:755:B:THR:H	2:756:B:ASN:H	11	0.12
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	14	0.12
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	1	0.12
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	2	0.12
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	6	0.12
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	9	0.12
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	7	0.12
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	9	0.12
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	17	0.12
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	4	0.12
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	10	0.12
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	14	0.12
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	16	0.12
(1,1861)	2:745:B:PRO:HD2	2:746:B:LEU:H	16	0.12
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	1	0.12
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	4	0.12
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	11	0.12
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	19	0.12
(1,1821)	2:742:B:ALA:HB1	2:743:B:ASN:HD22	16	0.12
(1,1821)	2:742:B:ALA:HB2	2:743:B:ASN:HD22	16	0.12
(1,1821)	2:742:B:ALA:HB3	2:743:B:ASN:HD22	16	0.12
(1,1811)	2:741:B:THR:HB	2:742:B:ALA:H	6	0.12
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	5	0.12
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	6	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	6	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	11	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	12	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	13	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	14	0.12
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	18	0.12
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	16	0.12
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	18	0.12
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	11	0.12
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	14	0.12
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	19	0.12
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	5	0.12
(1,1661)	2:730:B:PHE:HE1	2:734:B:ARG:HD3	11	0.12
(1,1658)	2:730:B:PHE:HB3	2:731:B:GLU:HG3	7	0.12
(1,1625)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	7	0.12
(1,1625)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	7	0.12
(1,1625)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	1	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	3	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	4	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	8	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	9	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	10	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	11	0.12
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	18	0.12
(1,1583)	2:725:B:LYS:HA	2:729:B:LYS:HE3	4	0.12
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	3	0.12
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	6	0.12
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	14	0.12
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	20	0.12
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	3	0.12
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	6	0.12
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	10	0.12
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	12	0.12
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	16	0.12
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	8	0.12
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	11	0.12
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	20	0.12
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	1	0.12
(1,1236)	2:709:B:LEU:H	2:711:B:ALA:H	14	0.12
(1,1235)	2:709:B:LEU:HB3	2:710:B:ALA:HA	20	0.12
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	11	0.12
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	20	0.12
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	5	0.12
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	17	0.12
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	12	0.12
(1,870)	2:693:B:ILE:H	2:693:B:ILE:HB	16	0.12
(1,864)	2:692:B:ASP:H	2:696:B:VAL:H	1	0.12
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	9	0.12
(1,848)	2:692:B:ASP:H	2:692:B:ASP:HB3	14	0.12
(1,848)	2:692:B:ASP:H	2:692:B:ASP:HB3	16	0.12
(1,820)	2:689:B:LYS:H	2:689:B:LYS:HB2	7	0.12
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	1	0.12
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	16	0.12
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	2	0.12
(1,802)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	13	0.12
(1,778)	1:1000:A:LEU:H	1:1000:A:LEU:HB3	15	0.12
(1,774)	1:999:A:PRO:HB2	1:1000:A:LEU:H	6	0.12
(1,760)	1:997:A:ARG:HA	1:999:A:PRO:HD3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:996:A:ASN:H	1:997:A:ARG:H	17	0.12
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	12	0.12
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	13	0.12
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	2	0.12
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	14	0.12
(1,724)	1:994:A:LYS:HB2	1:995:A:ARG:HG3	14	0.12
(1,718)	1:994:A:LYS:HB2	1:995:A:ARG:H	11	0.12
(1,707)	1:994:A:LYS:HE3	1:994:A:LYS:HG3	19	0.12
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	4	0.12
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	10	0.12
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	16	0.12
(1,697)	1:993:A:PHE:H	1:995:A:ARG:H	12	0.12
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	7	0.12
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	8	0.12
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	13	0.12
(1,638)	1:990:A:VAL:H	1:992:A:PHE:H	1	0.12
(1,611)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	11	0.12
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	2	0.12
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	6	0.12
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	13	0.12
(1,451)	1:984:A:VAL:H	1:987:A:MET:H	1	0.12
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	20	0.12
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	20	0.12
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	20	0.12
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	14	0.12
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	9	0.12
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	20	0.12
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	13	0.12
(1,331)	1:978:A:LEU:HA	1:981:A:THR:H	17	0.12
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	8	0.12
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	9	0.12
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	13	0.12
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	5	0.12
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	10	0.12
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	3	0.12
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	5	0.12
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	16	0.12
(1,189)	1:970:A:LEU:H	1:970:A:LEU:HB3	20	0.12
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	12	0.12
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	13	0.12
(1,183)	1:969:A:VAL:H	1:972:A:GLY:HA3	14	0.12
(1,175)	1:969:A:VAL:H	1:970:A:LEU:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	3	0.12
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	7	0.12
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	8	0.12
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	1	0.12
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	4	0.12
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	10	0.12
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	15	0.12
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	10	0.12
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	16	0.12
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	3	0.12
(1,63)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	2	0.12
(1,63)	1:965:A:PRO:HG3	1:967:A:TRP:HB2	6	0.12
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	15	0.12
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	18	0.12
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	7	0.12
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	10	0.12
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	14	0.12
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	17	0.12
(3,288)	2:716:B:LYS:O	2:720:B:THR:H	3	0.11
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	18	0.11
(3,225)	2:695:B:VAL:O	2:699:B:SER:H	17	0.11
(3,211)	1:984:A:VAL:O	1:987:A:MET:H	18	0.11
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	10	0.11
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	14	0.11
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	2	0.11
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	15	0.11
(3,129)	2:716:B:LYS:O	2:720:B:THR:H	3	0.11
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	18	0.11
(3,66)	2:695:B:VAL:O	2:699:B:SER:H	17	0.11
(3,52)	1:984:A:VAL:O	1:987:A:MET:H	18	0.11
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	10	0.11
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	14	0.11
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	2	0.11
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	15	0.11
(1,4162)	1:988:A:TRP:HE1	2:719:B:ILE:HB	11	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	8	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	8	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	8	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	10	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	10	0.11
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	10	0.11
(1,4157)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	9	0.11
(1,4156)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	10	0.11
(1,4151)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	13	0.11
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	2	0.11
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	10	0.11
(1,4093)	1:969:A:VAL:HA	2:700:B:VAL:H	12	0.11
(1,4093)	1:969:A:VAL:HA	2:700:B:VAL:H	20	0.11
(1,4085)	1:968:A:TRP:HE1	2:693:B:ILE:HB	5	0.11
(1,4079)	2:760:B:ARG:HD3	2:760:B:ARG:HB2	1	0.11
(1,4070)	2:759:B:TYR:H	2:759:B:TYR:HB2	20	0.11
(1,4066)	2:758:B:THR:HB	2:759:B:TYR:H	11	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD11	3	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD12	3	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD13	3	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD11	4	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD12	4	0.11
(1,4049)	2:756:B:ASN:H	2:757:B:ILE:HD13	4	0.11
(1,4040)	2:756:B:ASN:H	2:756:B:ASN:HB2	19	0.11
(1,4034)	2:755:B:THR:H	2:755:B:THR:HB	19	0.11
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	6	0.11
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	15	0.11
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	20	0.11
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	7	0.11
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	10	0.11
(1,4027)	2:753:B:THR:HA	2:754:B:PHE:H	19	0.11
(1,4013)	2:751:B:THR:H	2:752:B:SER:H	20	0.11
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	8	0.11
(1,4000)	2:749:B:GLU:H	2:749:B:GLU:HG3	11	0.11
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	2	0.11
(1,3968)	2:747:B:TYR:H	2:747:B:TYR:HB3	14	0.11
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	12	0.11
(1,3935)	2:744:B:ASN:HA	2:747:B:TYR:H	16	0.11
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	2	0.11
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	8	0.11
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	2	0.11
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	5	0.11
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	14	0.11
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	15	0.11
(1,3894)	2:741:B:THR:HB	2:742:B:ALA:H	1	0.11
(1,3888)	2:740:B:ASP:HA	2:741:B:THR:H	16	0.11
(1,3887)	2:740:B:ASP:HB3	2:741:B:THR:H	1	0.11
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	9	0.11
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	10	0.11
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	19	0.11
(1,3881)	2:739:B:TRP:HB3	2:740:B:ASP:H	20	0.11
(1,3872)	2:738:B:LYS:HA	2:741:B:THR:H	19	0.11
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	13	0.11
(1,3857)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	2	0.11
(1,3857)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	5	0.11
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	11	0.11
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	13	0.11
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	15	0.11
(1,3745)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	19	0.11
(1,3742)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	19	0.11
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	13	0.11
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	14	0.11
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	15	0.11
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	17	0.11
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	2	0.11
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	11	0.11
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	12	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	1	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	2	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	5	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	6	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	8	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	9	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	10	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	13	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	14	0.11
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	15	0.11
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	13	0.11
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	18	0.11
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	4	0.11
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	5	0.11
(1,3638)	2:724:B:ARG:HA	2:728:B:ALA:H	12	0.11
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	13	0.11
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	3	0.11
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	9	0.11
(1,3617)	2:724:B:ARG:H	2:724:B:ARG:HB3	17	0.11
(1,3579)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	8	0.11
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	4	0.11
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	4	0.11
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	8	0.11
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	8	0.11
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	8	0.11
(1,3553)	2:720:B:THR:HG21	2:724:B:ARG:HD3	18	0.11
(1,3553)	2:720:B:THR:HG22	2:724:B:ARG:HD3	18	0.11
(1,3553)	2:720:B:THR:HG23	2:724:B:ARG:HD3	18	0.11
(1,3508)	2:718:B:LEU:HD21	2:721:B:ILE:HB	19	0.11
(1,3508)	2:718:B:LEU:HD22	2:721:B:ILE:HB	19	0.11
(1,3508)	2:718:B:LEU:HD23	2:721:B:ILE:HB	19	0.11
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	9	0.11
(1,3495)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	16	0.11
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	9	0.11
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	12	0.11
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	13	0.11
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	19	0.11
(1,3356)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	20	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	1	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	2	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	5	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	6	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	8	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	10	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	13	0.11
(1,3185)	2:703:B:ALA:HA	2:706:B:LEU:HB3	19	0.11
(1,3148)	2:701:B:MET:HG3	2:704:B:ILE:HG13	2	0.11
(1,3073)	2:698:B:LEU:H	2:698:B:LEU:HB3	15	0.11
(1,3059)	2:697:B:LEU:HB3	2:699:B:SER:H	1	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	4	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	6	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	7	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	10	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	12	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	13	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	18	0.11
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	19	0.11
(1,2934)	2:692:B:ASP:H	2:693:B:ILE:H	14	0.11
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	2	0.11
(1,2933)	2:692:B:ASP:HA	2:693:B:ILE:H	18	0.11
(1,2932)	2:692:B:ASP:HB3	2:693:B:ILE:H	18	0.11
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	8	0.11
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	18	0.11
(1,2886)	1:1004:A:ASP:HA	1:1005:A:GLU:H	17	0.11
(1,2885)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	7	0.11
(1,2885)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	16	0.11
(1,2884)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	19	0.11
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	4	0.11
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	5	0.11
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	15	0.11
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	16	0.11
(1,2873)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	9	0.11
(1,2833)	1:996:A:ASN:HA	1:997:A:ARG:H	6	0.11
(1,2821)	1:995:A:ARG:HA	1:996:A:ASN:H	9	0.11
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	3	0.11
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	9	0.11
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	12	0.11
(1,2808)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	19	0.11
(1,2787)	1:994:A:LYS:H	1:994:A:LYS:HG3	1	0.11
(1,2784)	1:993:A:PHE:HA	1:996:A:ASN:H	15	0.11
(1,2780)	1:993:A:PHE:H	1:995:A:ARG:H	18	0.11
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	2	0.11
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	2	0.11
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	6	0.11
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	18	0.11
(1,2773)	1:993:A:PHE:HB2	1:994:A:LYS:H	19	0.11
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	3	0.11
(1,2767)	1:993:A:PHE:HB3	1:993:A:PHE:H	19	0.11
(1,2755)	1:992:A:PHE:HB3	1:993:A:PHE:H	6	0.11
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	3	0.11
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	12	0.11
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	19	0.11
(1,2721)	1:990:A:VAL:H	1:992:A:PHE:H	7	0.11
(1,2694)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	9	0.11
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	4	0.11
(1,2659)	1:989:A:LYS:H	1:989:A:LYS:HD3	16	0.11
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	1	0.11
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	4	0.11
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	9	0.11
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	3	0.11
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	5	0.11
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	12	0.11
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	17	0.11
(1,2631)	1:987:A:MET:HA	1:990:A:VAL:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2629)	1:987:A:MET:HA	1:989:A:LYS:H	15	0.11
(1,2571)	1:985:A:LEU:H	1:987:A:MET:HG3	10	0.11
(1,2534)	1:984:A:VAL:H	1:987:A:MET:H	12	0.11
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	2	0.11
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	2	0.11
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	2	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	1	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	3	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	9	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	12	0.11
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	17	0.11
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	2	0.11
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	12	0.11
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	6	0.11
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	15	0.11
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	16	0.11
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	7	0.11
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	9	0.11
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	12	0.11
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	2	0.11
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	15	0.11
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	17	0.11
(1,2313)	1:971:A:VAL:HA	1:974:A:LEU:HB3	20	0.11
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	16	0.11
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	12	0.11
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	1	0.11
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	12	0.11
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	6	0.11
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	11	0.11
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	17	0.11
(1,2194)	1:967:A:TRP:HB3	1:967:A:TRP:HZ3	14	0.11
(1,2187)	1:966:A:ILE:HA	1:970:A:LEU:H	6	0.11
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	10	0.11
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	15	0.11
(1,2173)	1:966:A:ILE:HB	1:967:A:TRP:H	8	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD11	15	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD12	15	0.11
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD13	15	0.11
(1,2094)	1:961:A:GLU:H	1:962:A:ARG:H	3	0.11
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	1	0.11
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	10	0.11
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:961:A:GLU:H	1:961:A:GLU:HB3	19	0.11
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	11	0.11
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	20	0.11
(1,2079)	1:988:A:TRP:HE1	2:719:B:ILE:HB	11	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	8	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	8	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	8	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	10	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	10	0.11
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	10	0.11
(1,2074)	1:988:A:TRP:HE1	2:715:B:TRP:HH2	2	0.11
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	9	0.11
(1,2073)	1:988:A:TRP:HE1	2:715:B:TRP:HD1	10	0.11
(1,2068)	1:985:A:LEU:HB2	2:715:B:TRP:HE1	13	0.11
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	2	0.11
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	10	0.11
(1,2010)	1:969:A:VAL:HA	2:700:B:VAL:H	12	0.11
(1,2010)	1:969:A:VAL:HA	2:700:B:VAL:H	20	0.11
(1,2002)	1:968:A:TRP:HE1	2:693:B:ILE:HB	5	0.11
(1,1996)	2:760:B:ARG:HD3	2:760:B:ARG:HB2	1	0.11
(1,1987)	2:759:B:TYR:H	2:759:B:TYR:HB2	20	0.11
(1,1983)	2:758:B:THR:HB	2:759:B:TYR:H	11	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD11	3	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD12	3	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD13	3	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD11	4	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD12	4	0.11
(1,1966)	2:756:B:ASN:H	2:757:B:ILE:HD13	4	0.11
(1,1957)	2:756:B:ASN:H	2:756:B:ASN:HB2	19	0.11
(1,1951)	2:755:B:THR:H	2:755:B:THR:HB	19	0.11
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	6	0.11
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	15	0.11
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	20	0.11
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	7	0.11
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	10	0.11
(1,1944)	2:753:B:THR:HA	2:754:B:PHE:H	19	0.11
(1,1930)	2:751:B:THR:H	2:752:B:SER:H	20	0.11
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	8	0.11
(1,1917)	2:749:B:GLU:H	2:749:B:GLU:HG3	11	0.11
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	2	0.11
(1,1885)	2:747:B:TYR:H	2:747:B:TYR:HB3	14	0.11
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1852)	2:744:B:ASN:HA	2:747:B:TYR:H	16	0.11
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	2	0.11
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	8	0.11
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	2	0.11
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	5	0.11
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	14	0.11
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	15	0.11
(1,1811)	2:741:B:THR:HB	2:742:B:ALA:H	1	0.11
(1,1805)	2:740:B:ASP:HA	2:741:B:THR:H	16	0.11
(1,1804)	2:740:B:ASP:HB3	2:741:B:THR:H	1	0.11
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	8	0.11
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	9	0.11
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	10	0.11
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	19	0.11
(1,1798)	2:739:B:TRP:HB3	2:740:B:ASP:H	20	0.11
(1,1789)	2:738:B:LYS:HA	2:741:B:THR:H	19	0.11
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	13	0.11
(1,1774)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	2	0.11
(1,1774)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	5	0.11
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	11	0.11
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	13	0.11
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	15	0.11
(1,1662)	2:730:B:PHE:HE1	2:734:B:ARG:HD2	19	0.11
(1,1659)	2:730:B:PHE:HB3	2:731:B:GLU:HG2	19	0.11
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	13	0.11
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	14	0.11
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	15	0.11
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	17	0.11
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	2	0.11
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	11	0.11
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	12	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	1	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	2	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	5	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	6	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	8	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	9	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	10	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	13	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	14	0.11
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	15	0.11
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	18	0.11
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	4	0.11
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	5	0.11
(1,1555)	2:724:B:ARG:HA	2:728:B:ALA:H	12	0.11
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	13	0.11
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	3	0.11
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	9	0.11
(1,1534)	2:724:B:ARG:H	2:724:B:ARG:HB3	17	0.11
(1,1496)	2:721:B:ILE:HG12	2:724:B:ARG:HG3	8	0.11
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	4	0.11
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	4	0.11
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	4	0.11
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	8	0.11
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	8	0.11
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	8	0.11
(1,1470)	2:720:B:THR:HG21	2:724:B:ARG:HD3	18	0.11
(1,1470)	2:720:B:THR:HG22	2:724:B:ARG:HD3	18	0.11
(1,1470)	2:720:B:THR:HG23	2:724:B:ARG:HD3	18	0.11
(1,1425)	2:718:B:LEU:HD21	2:721:B:ILE:HB	19	0.11
(1,1425)	2:718:B:LEU:HD22	2:721:B:ILE:HB	19	0.11
(1,1425)	2:718:B:LEU:HD23	2:721:B:ILE:HB	19	0.11
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	9	0.11
(1,1412)	2:718:B:LEU:HB3	2:719:B:ILE:HG12	16	0.11
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	9	0.11
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	12	0.11
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	13	0.11
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	19	0.11
(1,1273)	2:712:B:LEU:HB3	2:713:B:LEU:HB2	20	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	1	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	2	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	5	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	6	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	8	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	10	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	13	0.11
(1,1102)	2:703:B:ALA:HA	2:706:B:LEU:HB3	19	0.11
(1,1065)	2:701:B:MET:HG3	2:704:B:ILE:HG13	2	0.11
(1,990)	2:698:B:LEU:H	2:698:B:LEU:HB3	15	0.11
(1,976)	2:697:B:LEU:HB3	2:699:B:SER:H	1	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	4	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	6	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	10	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	12	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	13	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	18	0.11
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	19	0.11
(1,851)	2:692:B:ASP:H	2:693:B:ILE:H	14	0.11
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	2	0.11
(1,850)	2:692:B:ASP:HA	2:693:B:ILE:H	18	0.11
(1,849)	2:692:B:ASP:HB3	2:693:B:ILE:H	18	0.11
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	8	0.11
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	14	0.11
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	18	0.11
(1,803)	1:1004:A:ASP:HA	1:1005:A:GLU:H	17	0.11
(1,802)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	7	0.11
(1,802)	1:1004:A:ASP:H	1:1004:A:ASP:HB2	16	0.11
(1,801)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	19	0.11
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	4	0.11
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	5	0.11
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	15	0.11
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	16	0.11
(1,790)	1:1001:A:GLU:H	1:1001:A:GLU:HB2	9	0.11
(1,750)	1:996:A:ASN:HA	1:997:A:ARG:H	6	0.11
(1,738)	1:995:A:ARG:HA	1:996:A:ASN:H	9	0.11
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	3	0.11
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	9	0.11
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	12	0.11
(1,725)	1:994:A:LYS:HB3	1:995:A:ARG:HG3	19	0.11
(1,704)	1:994:A:LYS:H	1:994:A:LYS:HG3	1	0.11
(1,701)	1:993:A:PHE:HA	1:996:A:ASN:H	15	0.11
(1,697)	1:993:A:PHE:H	1:995:A:ARG:H	18	0.11
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	2	0.11
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	2	0.11
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	6	0.11
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	18	0.11
(1,690)	1:993:A:PHE:HB2	1:994:A:LYS:H	19	0.11
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	3	0.11
(1,684)	1:993:A:PHE:HB3	1:993:A:PHE:H	19	0.11
(1,672)	1:992:A:PHE:HB3	1:993:A:PHE:H	6	0.11
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	3	0.11
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	12	0.11
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	19	0.11
(1,638)	1:990:A:VAL:H	1:992:A:PHE:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:989:A:LYS:HE3	1:993:A:PHE:HE1	9	0.11
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	4	0.11
(1,576)	1:989:A:LYS:H	1:989:A:LYS:HD3	16	0.11
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	1	0.11
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	4	0.11
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	9	0.11
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	3	0.11
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	5	0.11
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	12	0.11
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	17	0.11
(1,548)	1:987:A:MET:HA	1:990:A:VAL:H	19	0.11
(1,546)	1:987:A:MET:HA	1:989:A:LYS:H	15	0.11
(1,488)	1:985:A:LEU:H	1:987:A:MET:HG3	10	0.11
(1,451)	1:984:A:VAL:H	1:987:A:MET:H	12	0.11
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	2	0.11
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	2	0.11
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	2	0.11
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	1	0.11
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	3	0.11
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	9	0.11
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	12	0.11
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	17	0.11
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	2	0.11
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	12	0.11
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	6	0.11
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	15	0.11
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	16	0.11
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	7	0.11
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	9	0.11
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	12	0.11
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	2	0.11
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	15	0.11
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	17	0.11
(1,230)	1:971:A:VAL:HA	1:974:A:LEU:HB3	20	0.11
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	16	0.11
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	12	0.11
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	1	0.11
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	12	0.11
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	6	0.11
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	11	0.11
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	17	0.11
(1,111)	1:967:A:TRP:HB3	1:967:A:TRP:HZ3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:966:A:ILE:HA	1:970:A:LEU:H	6	0.11
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	10	0.11
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	15	0.11
(1,90)	1:966:A:ILE:HB	1:967:A:TRP:H	8	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD11	15	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD12	15	0.11
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD13	15	0.11
(1,11)	1:961:A:GLU:H	1:962:A:ARG:H	3	0.11
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	1	0.11
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	10	0.11
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	13	0.11
(1,8)	1:961:A:GLU:H	1:961:A:GLU:HB3	19	0.11
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	11	0.11
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	20	0.11
(3,282)	2:714:B:ILE:O	2:718:B:LEU:H	11	0.1
(3,270)	2:710:B:ALA:O	2:714:B:ILE:H	14	0.1
(3,240)	2:700:B:VAL:O	2:704:B:ILE:H	8	0.1
(3,202)	1:981:A:THR:O	1:984:A:VAL:H	19	0.1
(3,183)	1:974:A:LEU:O	1:978:A:LEU:H	1	0.1
(3,123)	2:714:B:ILE:O	2:718:B:LEU:H	11	0.1
(3,111)	2:710:B:ALA:O	2:714:B:ILE:H	14	0.1
(3,81)	2:700:B:VAL:O	2:704:B:ILE:H	8	0.1
(3,43)	1:981:A:THR:O	1:984:A:VAL:H	19	0.1
(3,24)	1:974:A:LEU:O	1:978:A:LEU:H	1	0.1
(2,81)	2:700:B:VAL:O	2:703:B:ALA:N	8	0.1
(2,81)	2:700:B:VAL:O	2:703:B:ALA:N	19	0.1
(2,27)	2:700:B:VAL:O	2:703:B:ALA:N	8	0.1
(2,27)	2:700:B:VAL:O	2:703:B:ALA:N	19	0.1
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG21	20	0.1
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG22	20	0.1
(1,4160)	1:988:A:TRP:H	2:719:B:ILE:HG23	20	0.1
(1,4138)	1:980:A:LEU:HA	2:708:B:GLY:H	12	0.1
(1,4111)	1:974:A:LEU:H	2:704:B:ILE:HG13	6	0.1
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	11	0.1
(1,4101)	1:973:A:VAL:H	2:700:B:VAL:HA	20	0.1
(1,4085)	1:968:A:TRP:HE1	2:693:B:ILE:HB	17	0.1
(1,4038)	2:755:B:THR:H	2:756:B:ASN:H	3	0.1
(1,4032)	2:754:B:PHE:HB3	2:755:B:THR:H	5	0.1
(1,4013)	2:751:B:THR:H	2:752:B:SER:H	8	0.1
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	4	0.1
(1,4007)	2:750:B:ALA:H	2:751:B:THR:H	12	0.1
(1,3979)	2:747:B:TYR:HA	2:750:B:ALA:HB1	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	2:747:B:TYR:HA	2:750:B:ALA:HB2	13	0.1
(1,3979)	2:747:B:TYR:HA	2:750:B:ALA:HB3	13	0.1
(1,3960)	2:746:B:LEU:HD11	2:746:B:LEU:HA	12	0.1
(1,3960)	2:746:B:LEU:HD12	2:746:B:LEU:HA	12	0.1
(1,3960)	2:746:B:LEU:HD13	2:746:B:LEU:HA	12	0.1
(1,3955)	2:746:B:LEU:H	2:746:B:LEU:HG	5	0.1
(1,3954)	2:746:B:LEU:H	2:746:B:LEU:HB2	8	0.1
(1,3924)	2:744:B:ASN:HB3	2:744:B:ASN:HD21	17	0.1
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	10	0.1
(1,3921)	2:744:B:ASN:H	2:744:B:ASN:HB2	14	0.1
(1,3911)	2:743:B:ASN:HB3	2:743:B:ASN:H	10	0.1
(1,3897)	2:741:B:THR:HA	2:744:B:ASN:H	18	0.1
(1,3891)	2:741:B:THR:H	2:741:B:THR:HG21	17	0.1
(1,3891)	2:741:B:THR:H	2:741:B:THR:HG22	17	0.1
(1,3891)	2:741:B:THR:H	2:741:B:THR:HG23	17	0.1
(1,3869)	2:738:B:LYS:H	2:740:B:ASP:H	8	0.1
(1,3857)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	10	0.1
(1,3850)	2:738:B:LYS:HA	2:738:B:LYS:HD3	15	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	4	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	7	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	9	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	13	0.1
(1,3822)	2:736:B:ARG:H	2:736:B:ARG:HB3	14	0.1
(1,3795)	2:734:B:ARG:H	2:734:B:ARG:HB3	9	0.1
(1,3708)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	9	0.1
(1,3708)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	9	0.1
(1,3708)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	9	0.1
(1,3706)	2:728:B:ALA:H	2:730:B:PHE:H	6	0.1
(1,3668)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	5	0.1
(1,3664)	2:725:B:LYS:HA	2:728:B:ALA:H	10	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	3	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	4	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	7	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	11	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	12	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	16	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	17	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	18	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	19	0.1
(1,3655)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	20	0.1
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	4	0.1
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3648)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	19	0.1
(1,3620)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	2	0.1
(1,3615)	2:724:B:ARG:H	2:724:B:ARG:HG3	16	0.1
(1,3507)	2:718:B:LEU:HD11	2:721:B:ILE:HB	14	0.1
(1,3507)	2:718:B:LEU:HD12	2:721:B:ILE:HB	14	0.1
(1,3507)	2:718:B:LEU:HD13	2:721:B:ILE:HB	14	0.1
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	4	0.1
(1,3470)	2:717:B:LEU:H	2:719:B:ILE:H	14	0.1
(1,3321)	2:709:B:LEU:HA	2:712:B:LEU:HB2	12	0.1
(1,3073)	2:698:B:LEU:H	2:698:B:LEU:HB3	16	0.1
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	2	0.1
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	11	0.1
(1,3033)	2:696:B:VAL:H	2:696:B:VAL:HB	15	0.1
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	9	0.1
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	12	0.1
(1,2894)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	17	0.1
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	1	0.1
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	3	0.1
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	17	0.1
(1,2890)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	19	0.1
(1,2889)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	13	0.1
(1,2884)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	8	0.1
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	6	0.1
(1,2874)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	7	0.1
(1,2844)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	10	0.1
(1,2825)	1:996:A:ASN:H	1:996:A:ASN:HB2	8	0.1
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	15	0.1
(1,2812)	1:995:A:ARG:H	1:995:A:ARG:HB3	19	0.1
(1,2780)	1:993:A:PHE:H	1:995:A:ARG:H	3	0.1
(1,2776)	1:993:A:PHE:H	1:994:A:LYS:HD3	10	0.1
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	13	0.1
(1,2730)	1:991:A:GLY:H	1:992:A:PHE:H	20	0.1
(1,2721)	1:990:A:VAL:H	1:992:A:PHE:H	17	0.1
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	17	0.1
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	18	0.1
(1,2640)	1:988:A:TRP:H	1:988:A:TRP:HB3	20	0.1
(1,2559)	1:985:A:LEU:HB2	1:986:A:ALA:H	1	0.1
(1,2559)	1:985:A:LEU:HB2	1:986:A:ALA:H	7	0.1
(1,2534)	1:984:A:VAL:H	1:987:A:MET:H	11	0.1
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG11	6	0.1
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG12	6	0.1
(1,2520)	1:984:A:VAL:H	1:984:A:VAL:HG13	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2515)	1:983:A:LEU:HB2	1:987:A:MET:H	16	0.1
(1,2491)	1:983:A:LEU:H	1:983:A:LEU:HB3	10	0.1
(1,2478)	1:982:A:ILE:HA	1:985:A:LEU:HB3	17	0.1
(1,2404)	1:977:A:LEU:HB2	1:981:A:THR:H	6	0.1
(1,2396)	1:977:A:LEU:HB2	1:978:A:LEU:H	9	0.1
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	4	0.1
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	15	0.1
(1,2358)	1:974:A:LEU:HB2	1:975:A:GLY:H	17	0.1
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	7	0.1
(1,2308)	1:971:A:VAL:H	1:973:A:VAL:H	20	0.1
(1,2291)	1:970:A:LEU:HB3	1:974:A:LEU:H	9	0.1
(1,2238)	1:968:A:TRP:HA	1:971:A:VAL:H	2	0.1
(1,2215)	1:968:A:TRP:H	1:968:A:TRP:HB3	17	0.1
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	1	0.1
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	2	0.1
(1,2203)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	12	0.1
(1,2189)	1:967:A:TRP:H	1:967:A:TRP:HB3	15	0.1
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	9	0.1
(1,2182)	1:966:A:ILE:HA	1:969:A:VAL:H	16	0.1
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD11	8	0.1
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD12	8	0.1
(1,2167)	1:966:A:ILE:H	1:966:A:ILE:HD13	8	0.1
(1,2158)	1:965:A:PRO:HD2	1:968:A:TRP:HB2	6	0.1
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	1	0.1
(1,2090)	1:960:A:GLU:HB2	1:961:A:GLU:H	19	0.1
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG21	20	0.1
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG22	20	0.1
(1,2077)	1:988:A:TRP:H	2:719:B:ILE:HG23	20	0.1
(1,2055)	1:980:A:LEU:HA	2:708:B:GLY:H	12	0.1
(1,2028)	1:974:A:LEU:H	2:704:B:ILE:HG13	6	0.1
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	11	0.1
(1,2018)	1:973:A:VAL:H	2:700:B:VAL:HA	20	0.1
(1,2002)	1:968:A:TRP:HE1	2:693:B:ILE:HB	17	0.1
(1,1955)	2:755:B:THR:H	2:756:B:ASN:H	3	0.1
(1,1949)	2:754:B:PHE:HB3	2:755:B:THR:H	5	0.1
(1,1930)	2:751:B:THR:H	2:752:B:SER:H	8	0.1
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	4	0.1
(1,1924)	2:750:B:ALA:H	2:751:B:THR:H	12	0.1
(1,1896)	2:747:B:TYR:HA	2:750:B:ALA:HB1	13	0.1
(1,1896)	2:747:B:TYR:HA	2:750:B:ALA:HB2	13	0.1
(1,1896)	2:747:B:TYR:HA	2:750:B:ALA:HB3	13	0.1
(1,1877)	2:746:B:LEU:HD11	2:746:B:LEU:HA	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1877)	2:746:B:LEU:HD12	2:746:B:LEU:HA	12	0.1
(1,1877)	2:746:B:LEU:HD13	2:746:B:LEU:HA	12	0.1
(1,1872)	2:746:B:LEU:H	2:746:B:LEU:HG	5	0.1
(1,1871)	2:746:B:LEU:H	2:746:B:LEU:HB2	8	0.1
(1,1841)	2:744:B:ASN:HB3	2:744:B:ASN:HD21	17	0.1
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	10	0.1
(1,1838)	2:744:B:ASN:H	2:744:B:ASN:HB2	14	0.1
(1,1828)	2:743:B:ASN:HB3	2:743:B:ASN:H	10	0.1
(1,1814)	2:741:B:THR:HA	2:744:B:ASN:H	18	0.1
(1,1808)	2:741:B:THR:H	2:741:B:THR:HG21	17	0.1
(1,1808)	2:741:B:THR:H	2:741:B:THR:HG22	17	0.1
(1,1808)	2:741:B:THR:H	2:741:B:THR:HG23	17	0.1
(1,1786)	2:738:B:LYS:H	2:740:B:ASP:H	8	0.1
(1,1774)	2:738:B:LYS:HE3	2:738:B:LYS:HB3	10	0.1
(1,1767)	2:738:B:LYS:HA	2:738:B:LYS:HD3	15	0.1
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	4	0.1
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	7	0.1
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	9	0.1
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	13	0.1
(1,1739)	2:736:B:ARG:H	2:736:B:ARG:HB3	14	0.1
(1,1712)	2:734:B:ARG:H	2:734:B:ARG:HB3	9	0.1
(1,1625)	2:728:B:ALA:HB1	2:731:B:GLU:HG2	9	0.1
(1,1625)	2:728:B:ALA:HB2	2:731:B:GLU:HG2	9	0.1
(1,1625)	2:728:B:ALA:HB3	2:731:B:GLU:HG2	9	0.1
(1,1623)	2:728:B:ALA:H	2:730:B:PHE:H	6	0.1
(1,1585)	2:725:B:LYS:HG3	2:729:B:LYS:HE3	5	0.1
(1,1581)	2:725:B:LYS:HA	2:728:B:ALA:H	10	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	3	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	4	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	7	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	11	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	12	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	16	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	17	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	18	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	19	0.1
(1,1572)	2:725:B:LYS:HD3	2:725:B:LYS:HB3	20	0.1
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	4	0.1
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	17	0.1
(1,1565)	2:725:B:LYS:HE3	2:725:B:LYS:HG3	19	0.1
(1,1537)	2:724:B:ARG:HD3	2:724:B:ARG:HB3	2	0.1
(1,1532)	2:724:B:ARG:H	2:724:B:ARG:HG3	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	2:718:B:LEU:HD11	2:721:B:ILE:HB	14	0.1
(1,1424)	2:718:B:LEU:HD12	2:721:B:ILE:HB	14	0.1
(1,1424)	2:718:B:LEU:HD13	2:721:B:ILE:HB	14	0.1
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	4	0.1
(1,1387)	2:717:B:LEU:H	2:719:B:ILE:H	14	0.1
(1,1238)	2:709:B:LEU:HA	2:712:B:LEU:HB2	12	0.1
(1,990)	2:698:B:LEU:H	2:698:B:LEU:HB3	16	0.1
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	2	0.1
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	11	0.1
(1,950)	2:696:B:VAL:H	2:696:B:VAL:HB	15	0.1
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	9	0.1
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	12	0.1
(1,811)	1:1006:A:GLU:H	1:1006:A:GLU:HB3	17	0.1
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	1	0.1
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	3	0.1
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	17	0.1
(1,807)	1:1005:A:GLU:H	1:1005:A:GLU:HB3	19	0.1
(1,806)	1:1005:A:GLU:H	1:1005:A:GLU:HB2	13	0.1
(1,801)	1:1004:A:ASP:H	1:1004:A:ASP:HB3	8	0.1
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	6	0.1
(1,791)	1:1002:A:GLU:H	1:1002:A:GLU:HB3	7	0.1
(1,761)	1:997:A:ARG:HD3	1:999:A:PRO:HG3	10	0.1
(1,742)	1:996:A:ASN:H	1:996:A:ASN:HB2	8	0.1
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	15	0.1
(1,729)	1:995:A:ARG:H	1:995:A:ARG:HB3	19	0.1
(1,697)	1:993:A:PHE:H	1:995:A:ARG:H	3	0.1
(1,693)	1:993:A:PHE:H	1:994:A:LYS:HD3	10	0.1
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	13	0.1
(1,647)	1:991:A:GLY:H	1:992:A:PHE:H	20	0.1
(1,638)	1:990:A:VAL:H	1:992:A:PHE:H	17	0.1
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	17	0.1
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	18	0.1
(1,557)	1:988:A:TRP:H	1:988:A:TRP:HB3	20	0.1
(1,476)	1:985:A:LEU:HB2	1:986:A:ALA:H	1	0.1
(1,476)	1:985:A:LEU:HB2	1:986:A:ALA:H	7	0.1
(1,451)	1:984:A:VAL:H	1:987:A:MET:H	11	0.1
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG11	6	0.1
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG12	6	0.1
(1,437)	1:984:A:VAL:H	1:984:A:VAL:HG13	6	0.1
(1,432)	1:983:A:LEU:HB2	1:987:A:MET:H	16	0.1
(1,408)	1:983:A:LEU:H	1:983:A:LEU:HB3	10	0.1
(1,395)	1:982:A:ILE:HA	1:985:A:LEU:HB3	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:977:A:LEU:HB2	1:981:A:THR:H	6	0.1
(1,313)	1:977:A:LEU:HB2	1:978:A:LEU:H	9	0.1
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	4	0.1
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	15	0.1
(1,275)	1:974:A:LEU:HB2	1:975:A:GLY:H	17	0.1
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	7	0.1
(1,225)	1:971:A:VAL:H	1:973:A:VAL:H	20	0.1
(1,208)	1:970:A:LEU:HB3	1:974:A:LEU:H	9	0.1
(1,155)	1:968:A:TRP:HA	1:971:A:VAL:H	2	0.1
(1,132)	1:968:A:TRP:H	1:968:A:TRP:HB3	17	0.1
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	1	0.1
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	2	0.1
(1,120)	1:967:A:TRP:HB3	1:968:A:TRP:HB3	12	0.1
(1,106)	1:967:A:TRP:H	1:967:A:TRP:HB3	15	0.1
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	9	0.1
(1,99)	1:966:A:ILE:HA	1:969:A:VAL:H	16	0.1
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD11	8	0.1
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD12	8	0.1
(1,84)	1:966:A:ILE:H	1:966:A:ILE:HD13	8	0.1
(1,75)	1:965:A:PRO:HD2	1:968:A:TRP:HB2	6	0.1
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	1	0.1
(1,7)	1:960:A:GLU:HB2	1:961:A:GLU:H	19	0.1

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

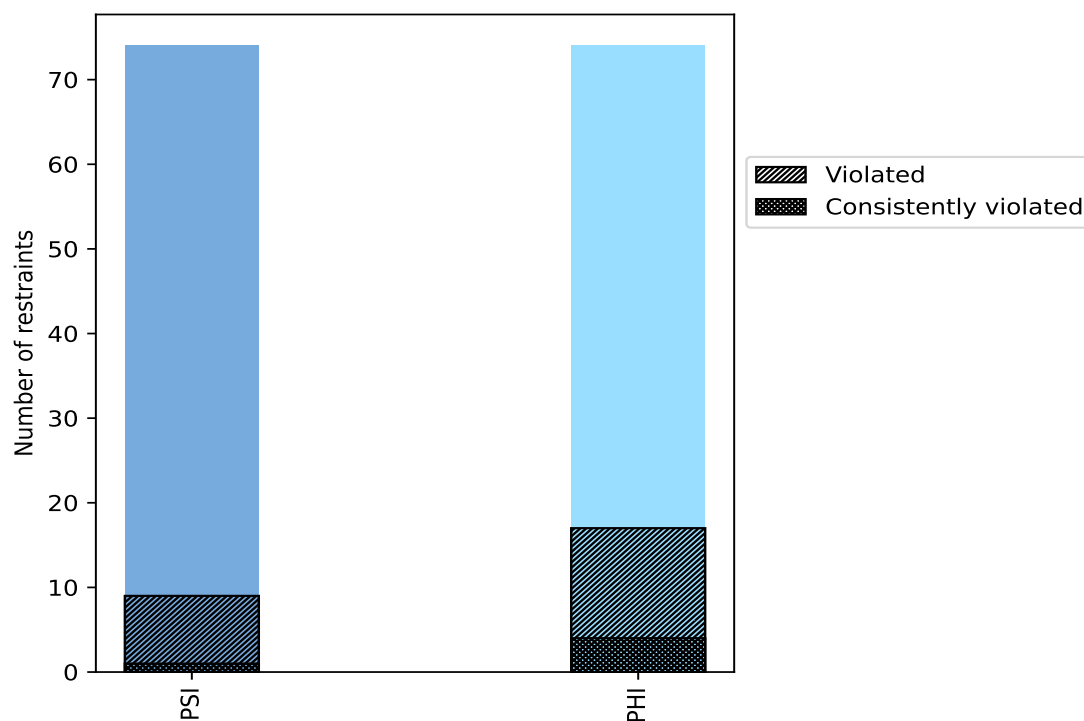
10.1 Summary of dihedral-angle violations [i](#)

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	74	50.0	9	12.2	6.1	1	1.4	0.7
PHI	74	50.0	17	23.0	11.5	4	5.4	2.7
Total	148	100.0	26	17.6	17.6	5	3.4	3.4

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](#)



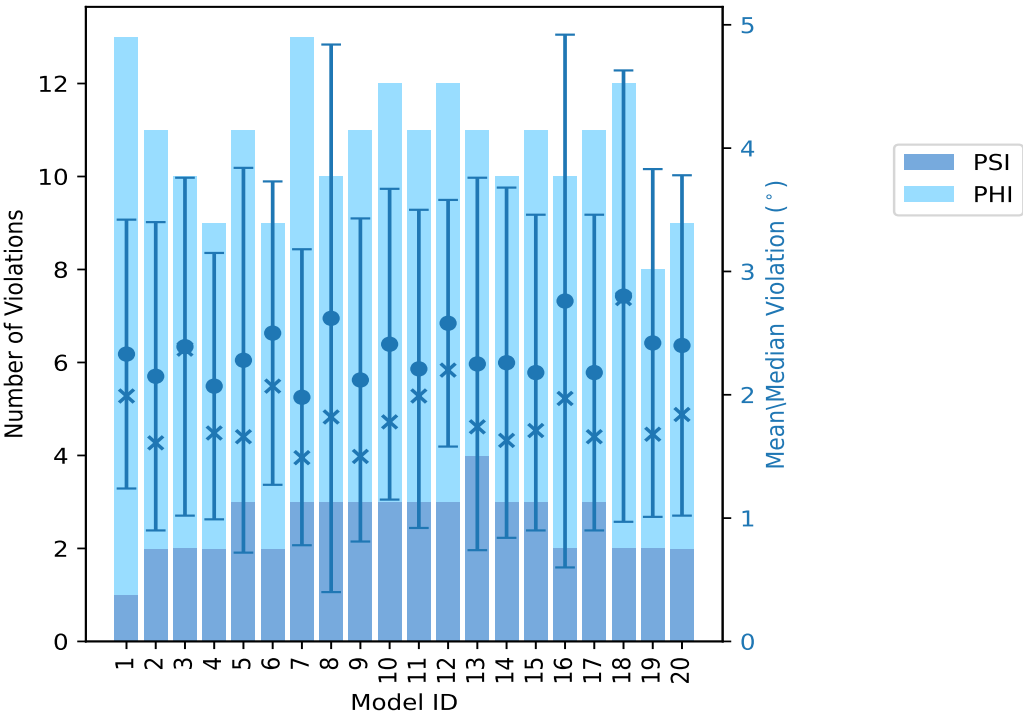
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	12	13	2.33	4.96	1.09	1.99
2	2	9	11	2.15	5.59	1.25	1.61
3	2	8	10	2.39	6.03	1.37	2.37
4	2	7	9	2.07	4.91	1.08	1.69
5	3	8	11	2.28	6.31	1.56	1.66
6	2	7	9	2.5	5.34	1.23	2.07
7	3	10	13	1.98	5.56	1.2	1.49
8	3	7	10	2.62	9.09	2.22	1.82
9	3	8	11	2.12	5.51	1.31	1.5
10	3	9	12	2.41	5.36	1.26	1.78
11	3	8	11	2.21	5.78	1.29	1.99
12	3	9	12	2.58	5.07	1.0	2.2
13	4	7	11	2.25	6.77	1.51	1.74
14	3	7	10	2.26	6.01	1.42	1.63
15	3	8	11	2.18	5.75	1.28	1.71
16	2	8	10	2.76	8.79	2.16	1.97
17	3	8	11	2.18	5.75	1.28	1.66
18	2	10	12	2.8	7.9	1.83	2.78
19	2	6	8	2.42	5.94	1.41	1.68
20	2	7	9	2.4	5.95	1.38	1.84

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



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

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

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

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

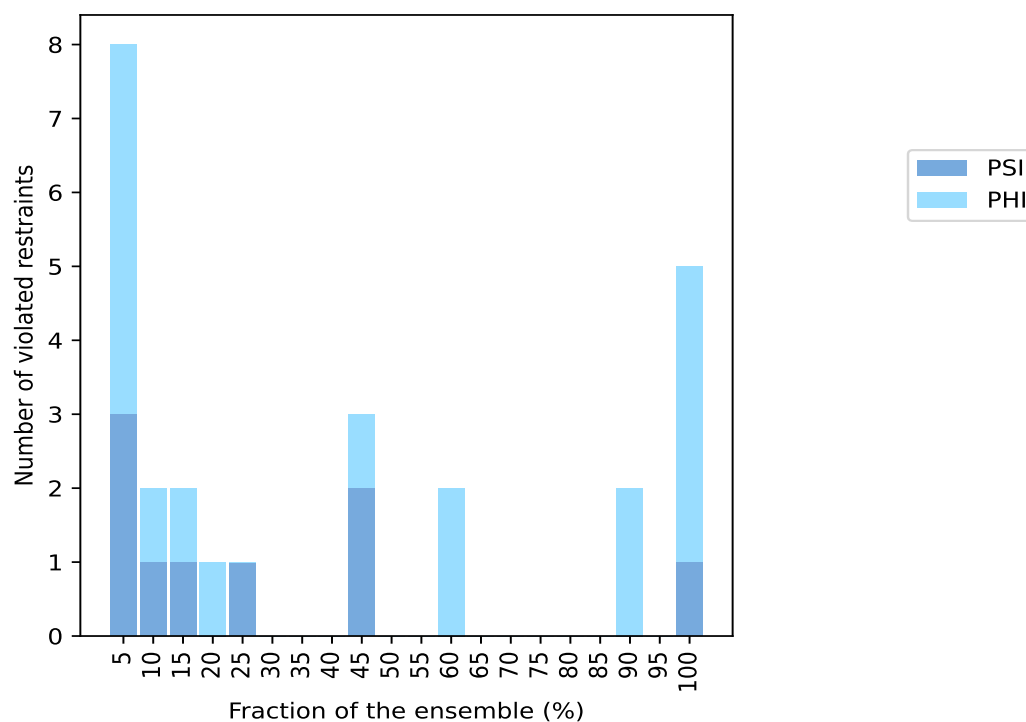
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	2	2	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	2	2	18	90.0
0	0	0	19	95.0
1	4	5	20	100.0

¹ Number of models with violations

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

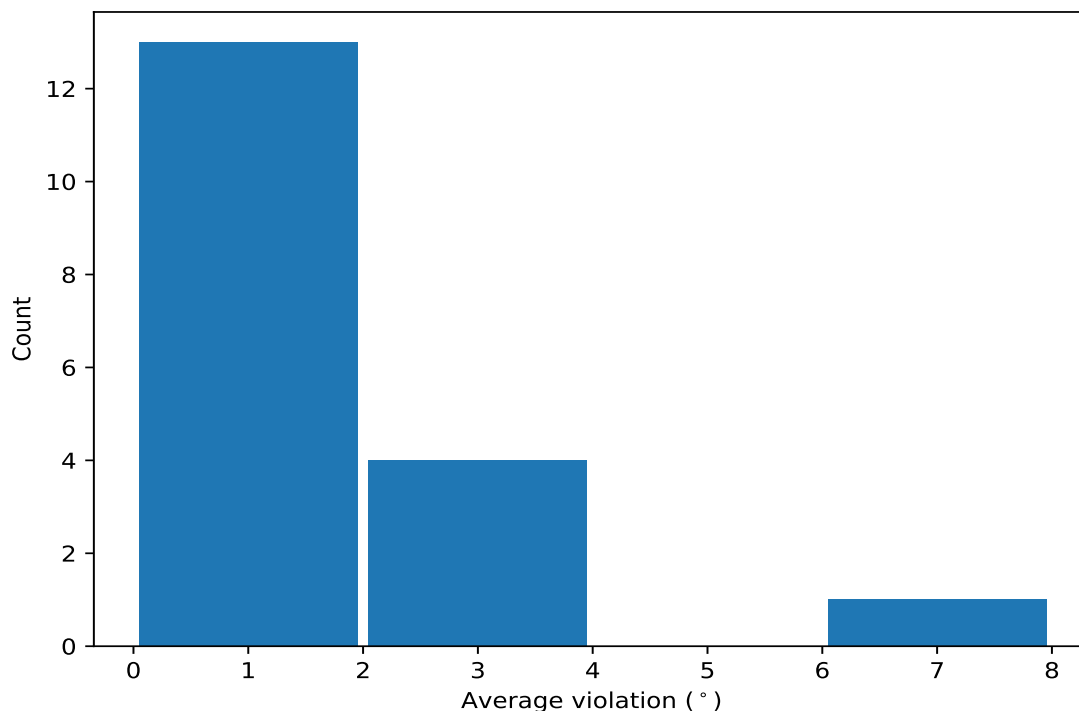


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

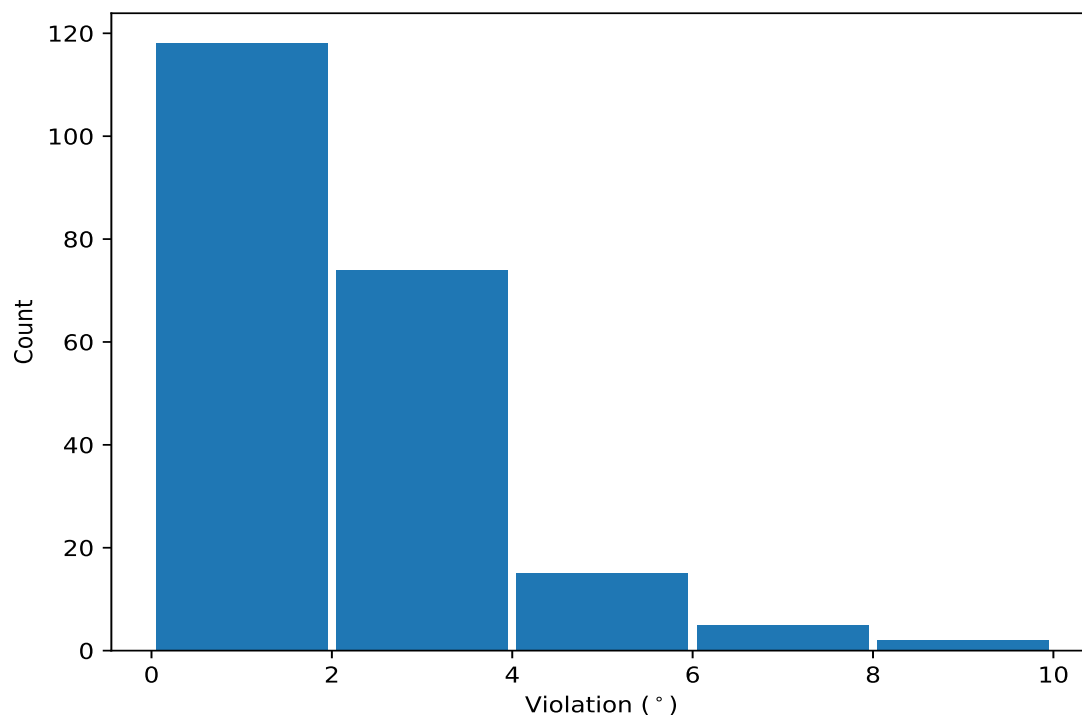
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	20	6.12	1.14	5.76
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	20	2.97	0.49	3.03
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	20	2.55	0.47	2.6
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	20	2.52	0.36	2.54
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	20	1.62	0.25	1.59
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	18	1.88	0.51	1.84
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	18	1.83	0.7	1.68
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	12	2.26	0.96	2.02
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	12	1.45	0.35	1.34
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	9	1.42	0.33	1.3
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	9	1.35	0.23	1.32
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	9	1.29	0.22	1.29
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	5	1.36	0.19	1.39
(1,33)	1:981:A:THR:C	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	4	1.4	0.17	1.38
(1,81)	2:707:B:ILE:C	2:708:B:GLY:N	2:708:B:GLY:CA	2:708:B:GLY:C	3	1.17	0.11	1.24
(1,126)	2:730:B:PHE:N	2:730:B:PHE:CA	2:730:B:PHE:C	2:731:B:GLU:N	3	1.15	0.11	1.23
(1,68)	2:700:B:VAL:N	2:700:B:VAL:CA	2:700:B:VAL:C	2:701:B:MET:N	2	1.32	0.07	1.32
(1,31)	1:980:A:LEU:C	1:981:A:THR:N	1:981:A:THR:CA	1:981:A:THR:C	2	1.02	0.02	1.02

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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 (°)
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	8	9.09
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	16	8.79
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	18	7.9
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	13	6.77
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	5	6.31
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	3	6.03
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	14	6.01
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	20	5.95
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	19	5.94
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	11	5.78
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	15	5.75
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	17	5.75
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	2	5.59
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	7	5.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	9	5.51
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	10	5.36
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	6	5.34
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	12	5.07
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	1	4.96
(1,39)	1:984:A:VAL:C	1:985:A:LEU:N	1:985:A:LEU:CA	1:985:A:LEU:C	4	4.91
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	18	4.27
(1,37)	1:983:A:LEU:C	1:984:A:VAL:N	1:984:A:VAL:CA	1:984:A:VAL:C	1	4.15
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	10	3.99
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	5	3.96
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	6	3.78
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	16	3.55
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	12	3.44
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	10	3.39
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	12	3.29
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	7	3.23
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	18	3.2
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	14	3.17
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	15	3.17
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	18	3.16
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	5	3.11
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	1	3.09
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	12	3.08
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	11	3.07
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	16	3.06
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	10	3.06
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	20	2.99
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	9	2.98
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	9	2.98
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	8	2.93
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	9	2.93
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	17	2.93
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	18	2.92
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	16	2.92
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	12	2.91
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	2	2.88
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	19	2.87
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	3	2.82
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	18	2.82
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	3	2.8
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	20	2.79
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	8	2.76
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	2	2.74
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	14	2.73
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	18	2.73
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	15	2.72
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	2	2.66
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	10	2.66
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	13	2.66
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	1	2.6
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	6	2.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	19	2.5
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	17	2.49
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	17	2.47
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	14	2.47
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	11	2.46
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	13	2.45
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	4	2.44
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	6	2.44
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	3	2.39
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	3	2.38
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	5	2.36
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	17	2.36
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	11	2.36
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	3	2.35
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	7	2.31
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	11	2.29
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	1	2.27
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	7	2.25
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	13	2.25
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	12	2.24
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	15	2.19
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	12	2.17
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	4	2.16
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	12	2.14
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	20	2.12
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	13	2.09
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	18	2.07
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	6	2.07
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	16	2.03
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	4	2.02
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	1	2.0
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	1	1.99
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	11	1.99
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	7	1.99
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	8	1.97
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	12	1.96
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	6	1.95
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	5	1.93
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	10	1.93
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	8	1.91
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	16	1.91
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	1	1.87
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	20	1.84
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	20	1.78
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	1	1.76
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	15	1.76
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	1	1.76
(1,88)	2:711:B:ALA:N	2:711:B:ALA:CA	2:711:B:ALA:C	2:712:B:LEU:N	12	1.75
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	13	1.74
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	8	1.73
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	7	1.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	15	1.71
(1,143)	2:738:B:LYS:C	2:739:B:TRP:N	2:739:B:TRP:CA	2:739:B:TRP:C	4	1.69
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	19	1.69
(1,116)	2:725:B:LYS:N	2:725:B:LYS:CA	2:725:B:LYS:C	2:726:B:GLU:N	19	1.68
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	3	1.68
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	2	1.67
(1,11)	1:970:A:LEU:C	1:971:A:VAL:N	1:971:A:VAL:CA	1:971:A:VAL:C	11	1.67
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	5	1.66
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	17	1.66
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	14	1.65
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	12	1.65
(1,33)	1:981:A:THR:C	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	10	1.64
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	9	1.63
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	14	1.61
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	2	1.61
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	19	1.6
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	10	1.58
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	15	1.58
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	19	1.57
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	13	1.56
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	16	1.56
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	20	1.56
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	10	1.56
(1,104)	2:719:B:ILE:N	2:719:B:ILE:CA	2:719:B:ILE:C	2:720:B:THR:N	18	1.54
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	4	1.54
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	2	1.53
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	13	1.53
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	6	1.52
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	17	1.5
(1,33)	1:981:A:THR:C	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	9	1.5
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	7	1.49
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	19	1.49
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	8	1.48
(1,105)	2:719:B:ILE:C	2:720:B:THR:N	2:720:B:THR:CA	2:720:B:THR:C	15	1.47
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	8	1.47
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	8	1.46
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	6	1.44
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	14	1.44
(1,103)	2:718:B:LEU:C	2:719:B:ILE:N	2:719:B:ILE:CA	2:719:B:ILE:C	1	1.44
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	10	1.44
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	13	1.4
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	17	1.39
(1,68)	2:700:B:VAL:N	2:700:B:VAL:CA	2:700:B:VAL:C	2:701:B:MET:N	8	1.39
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	9	1.39
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	2	1.38
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	6	1.38
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	4	1.37
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	15	1.37
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	5	1.33
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	20	1.32
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	3	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	16	1.31
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	10	1.3
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	7	1.3
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	4	1.3
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	2	1.29
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	14	1.29
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	15	1.27
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	5	1.25
(1,81)	2:707:B:ILE:C	2:708:B:GLY:N	2:708:B:GLY:CA	2:708:B:GLY:C	1	1.25
(1,68)	2:700:B:VAL:N	2:700:B:VAL:CA	2:700:B:VAL:C	2:701:B:MET:N	16	1.25
(1,33)	1:981:A:THR:C	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	2	1.25
(1,81)	2:707:B:ILE:C	2:708:B:GLY:N	2:708:B:GLY:CA	2:708:B:GLY:C	12	1.24
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	9	1.24
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	4	1.24
(1,126)	2:730:B:PHE:N	2:730:B:PHE:CA	2:730:B:PHE:C	2:731:B:GLU:N	11	1.23
(1,126)	2:730:B:PHE:N	2:730:B:PHE:CA	2:730:B:PHE:C	2:731:B:GLU:N	13	1.23
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	7	1.23
(1,33)	1:981:A:THR:C	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	11	1.23
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	7	1.22
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	14	1.22
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	20	1.22
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	7	1.19
(1,49)	1:989:A:LYS:C	1:990:A:VAL:N	1:990:A:VAL:CA	1:990:A:VAL:C	17	1.19
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	16	1.18
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	17	1.17
(1,111)	2:722:B:HIS:C	2:723:B:ASP:N	2:723:B:ASP:CA	2:723:B:ASP:C	9	1.16
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	3	1.15
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	1	1.14
(1,57)	2:694:B:LEU:C	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	7	1.12
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	11	1.11
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	7	1.1
(1,55)	2:693:B:ILE:C	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	17	1.09
(1,90)	2:712:B:LEU:N	2:712:B:LEU:CA	2:712:B:LEU:C	2:713:B:LEU:N	11	1.07
(1,29)	1:979:A:LEU:C	1:980:A:LEU:N	1:980:A:LEU:CA	1:980:A:LEU:C	5	1.07
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	5	1.06
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	13	1.04
(1,31)	1:980:A:LEU:C	1:981:A:THR:N	1:981:A:THR:CA	1:981:A:THR:C	5	1.04
(1,58)	2:695:B:VAL:N	2:695:B:VAL:CA	2:695:B:VAL:C	2:696:B:VAL:N	3	1.03
(1,81)	2:707:B:ILE:C	2:708:B:GLY:N	2:708:B:GLY:CA	2:708:B:GLY:C	18	1.02
(1,43)	1:986:A:ALA:C	1:987:A:MET:N	1:987:A:MET:CA	1:987:A:MET:C	9	1.02
(1,73)	2:703:B:ALA:C	2:704:B:ILE:N	2:704:B:ILE:CA	2:704:B:ILE:C	9	1.01
(1,56)	2:694:B:LEU:N	2:694:B:LEU:CA	2:694:B:LEU:C	2:695:B:VAL:N	10	1.01
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	2	1.01
(1,34)	1:982:A:ILE:N	1:982:A:ILE:CA	1:982:A:ILE:C	1:983:A:LEU:N	15	1.01
(1,13)	1:971:A:VAL:C	1:972:A:GLY:N	1:972:A:GLY:CA	1:972:A:GLY:C	18	1.01
(1,126)	2:730:B:PHE:N	2:730:B:PHE:CA	2:730:B:PHE:C	2:731:B:GLU:N	14	1.0
(1,31)	1:980:A:LEU:C	1:981:A:THR:N	1:981:A:THR:CA	1:981:A:THR:C	18	1.0