



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 02:23 pm BST

PDB ID : 5NOC
BMRB ID : 34122
Title : Solution NMR Structure of the C-terminal domain of ParB (Spo0J)
Authors : Higman, V.A.; Fisher, G.L.M.; Dillingham, M.S.; Crump, M.P.
Deposited on : 2017-04-11

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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.33

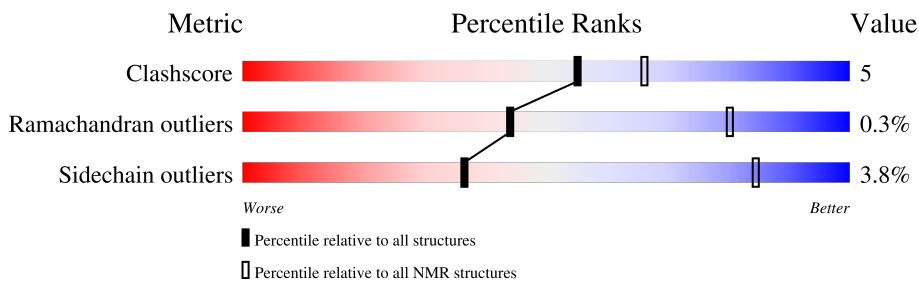
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	69	 68% 9% 22%
1	B	69	 70% 9% 22%

2 Ensemble composition and analysis i

This entry contains 20 models. Model 13 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:230-A:282, B:229-B:282 (107)	0.65	13

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1838 atoms, of which 928 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stage 0 sporulation protein J.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	54	919	287	464	78	90	0
1	B	54	919	287	464	78	90	0

There are 6 discrepancies between the modelled and reference sequences:

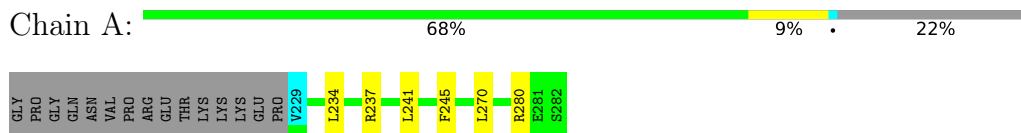
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	GLY	-	expression tag	UNP P26497
A	215	PRO	-	expression tag	UNP P26497
A	216	GLY	-	expression tag	UNP P26497
B	214	GLY	-	expression tag	UNP P26497
B	215	PRO	-	expression tag	UNP P26497
B	216	GLY	-	expression tag	UNP P26497

4 Residue-property plots [i](#)

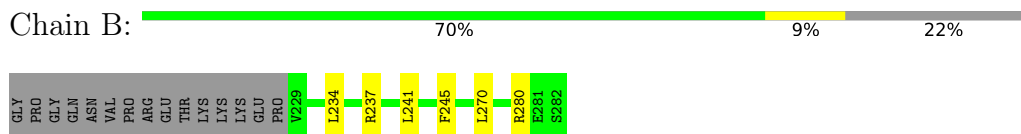
4.1 Average score per residue in the NMR ensemble

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: Stage 0 sporulation protein J



- Molecule 1: Stage 0 sporulation protein J

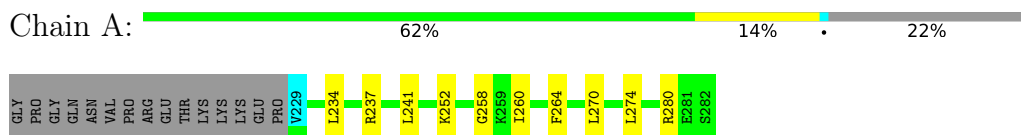


4.2 Scores per residue for each member of the ensemble

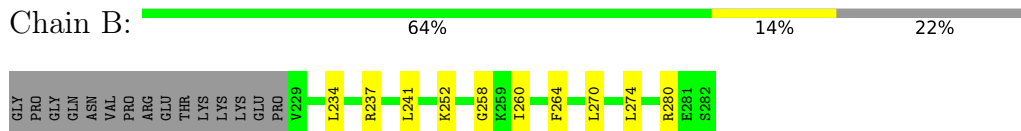
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Stage 0 sporulation protein J

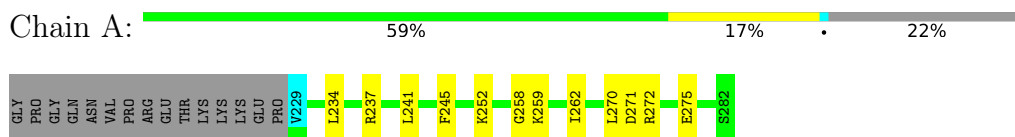


- Molecule 1: Stage 0 sporulation protein J

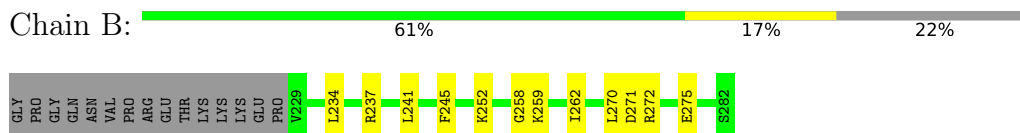


4.2.2 Score per residue for model 2

- Molecule 1: Stage 0 sporulation protein J

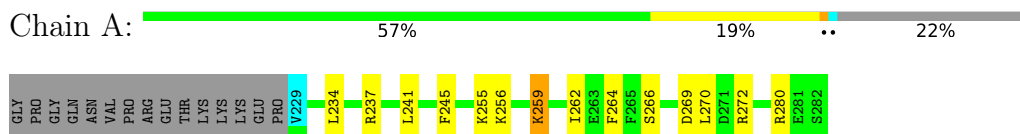


- Molecule 1: Stage 0 sporulation protein J

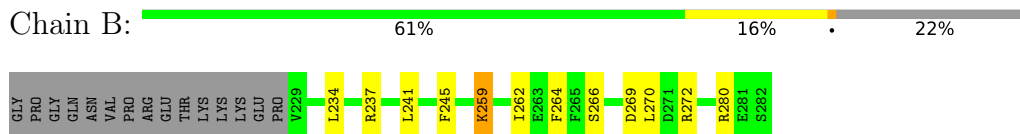


4.2.3 Score per residue for model 3

- Molecule 1: Stage 0 sporulation protein J

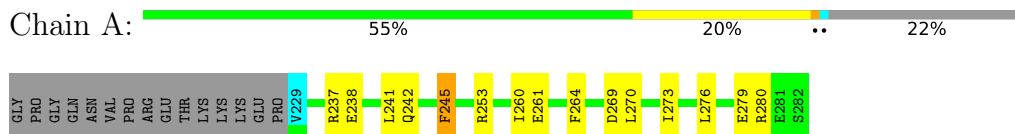


- Molecule 1: Stage 0 sporulation protein J

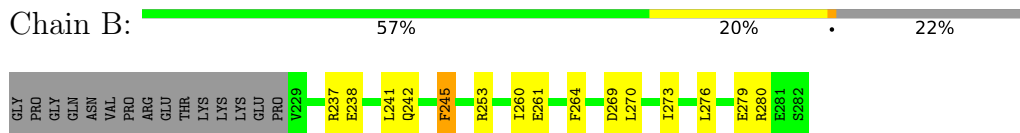


4.2.4 Score per residue for model 4

- Molecule 1: Stage 0 sporulation protein J

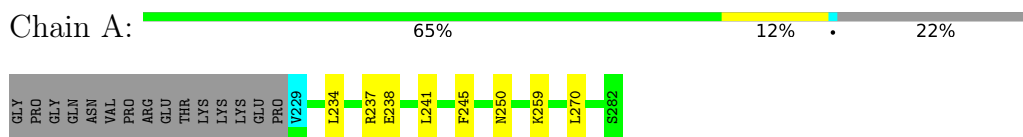


- Molecule 1: Stage 0 sporulation protein J

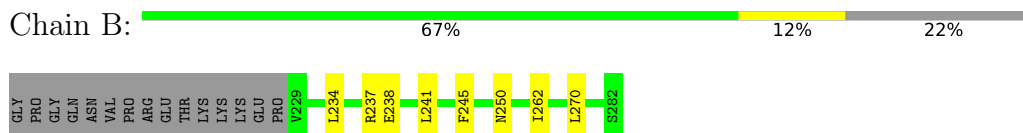


4.2.5 Score per residue for model 5

- Molecule 1: Stage 0 sporulation protein J

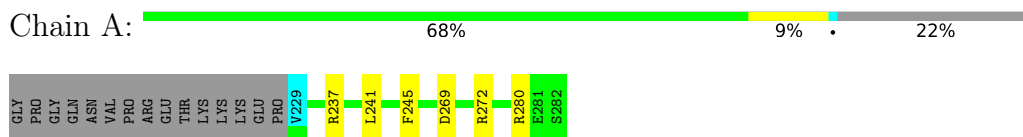


- Molecule 1: Stage 0 sporulation protein J

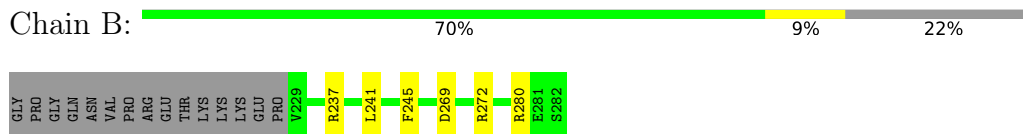


4.2.6 Score per residue for model 6

- Molecule 1: Stage 0 sporulation protein J

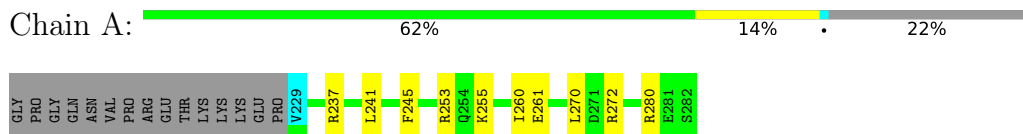


- Molecule 1: Stage 0 sporulation protein J

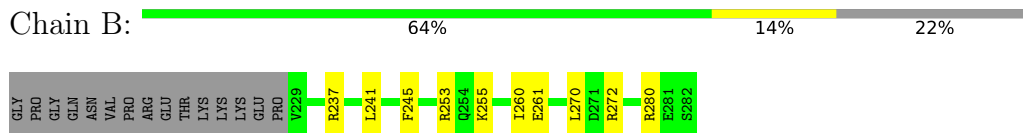


4.2.7 Score per residue for model 7

- Molecule 1: Stage 0 sporulation protein J

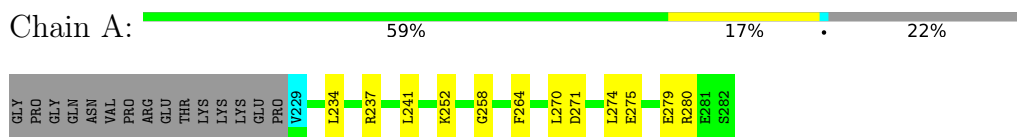


- Molecule 1: Stage 0 sporulation protein J

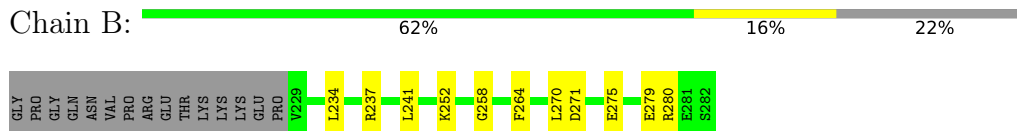


4.2.8 Score per residue for model 8

- Molecule 1: Stage 0 sporulation protein J

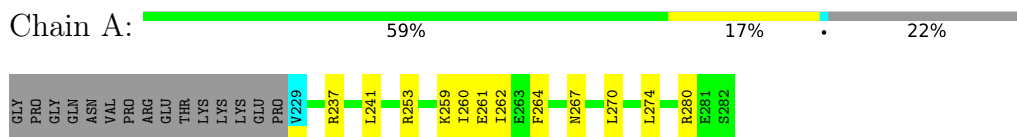


- Molecule 1: Stage 0 sporulation protein J

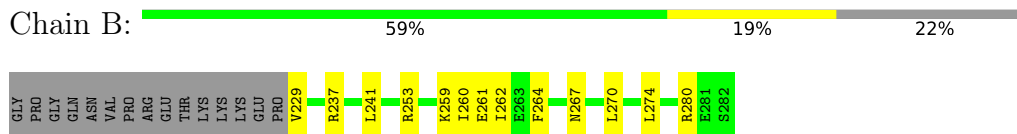


4.2.9 Score per residue for model 9

- Molecule 1: Stage 0 sporulation protein J

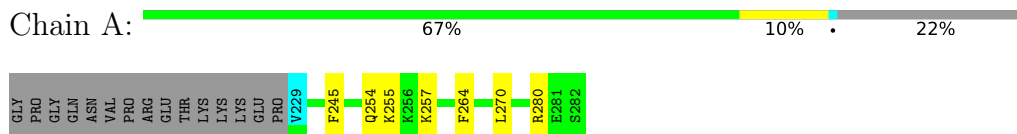


- Molecule 1: Stage 0 sporulation protein J

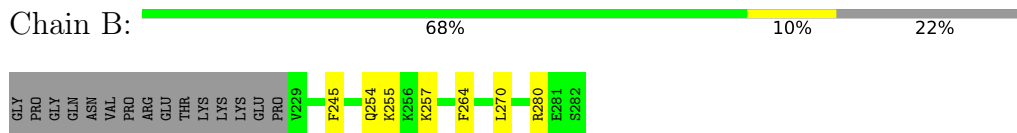


4.2.10 Score per residue for model 10

- Molecule 1: Stage 0 sporulation protein J

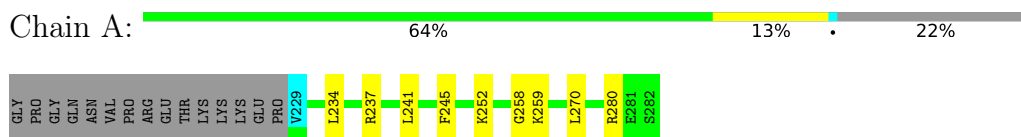


- Molecule 1: Stage 0 sporulation protein J

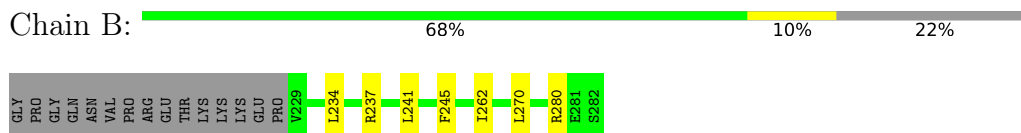


4.2.11 Score per residue for model 11

- Molecule 1: Stage 0 sporulation protein J

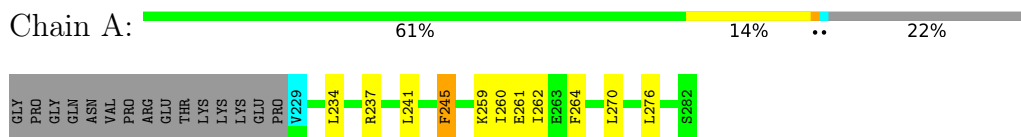


- Molecule 1: Stage 0 sporulation protein J

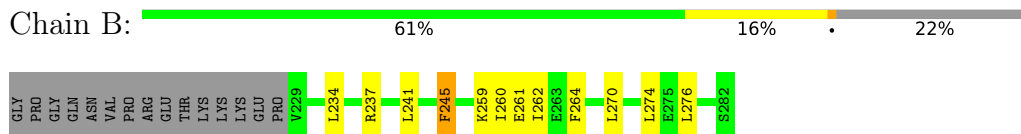


4.2.12 Score per residue for model 12

- Molecule 1: Stage 0 sporulation protein J

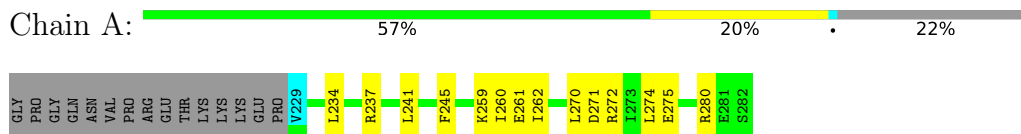


- Molecule 1: Stage 0 sporulation protein J

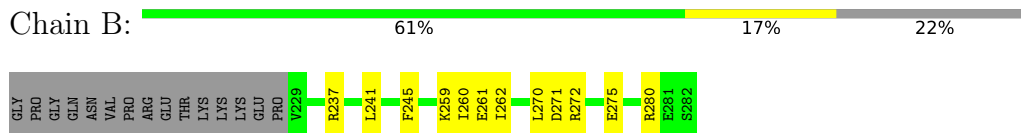


4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Stage 0 sporulation protein J

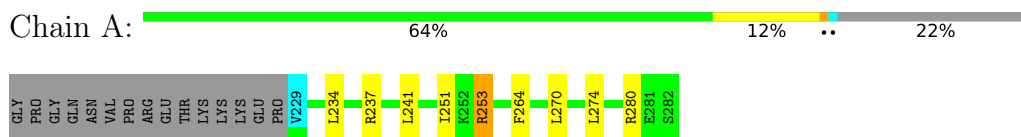


- Molecule 1: Stage 0 sporulation protein J

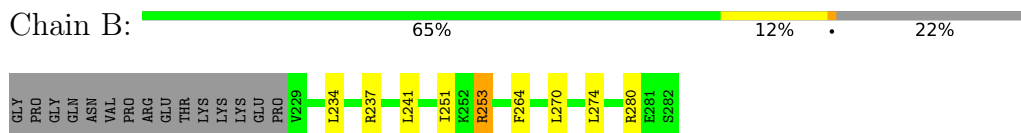


4.2.17 Score per residue for model 17

- Molecule 1: Stage 0 sporulation protein J

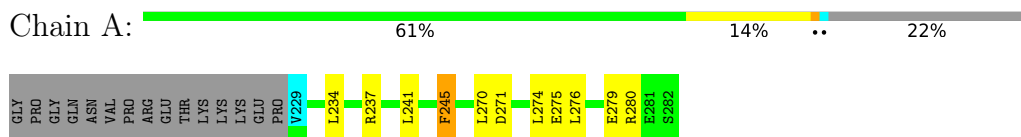


- Molecule 1: Stage 0 sporulation protein J

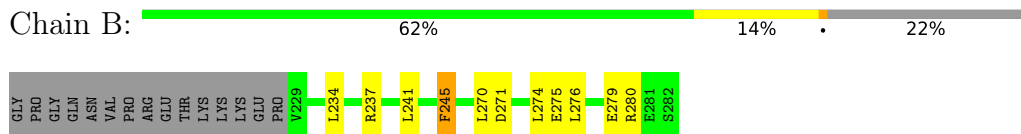


4.2.18 Score per residue for model 18

- Molecule 1: Stage 0 sporulation protein J

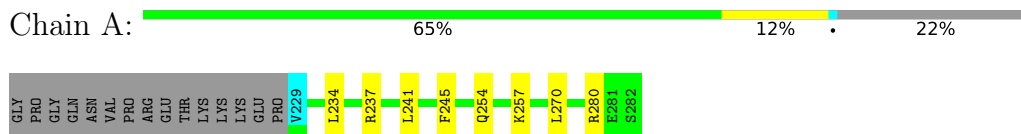


- Molecule 1: Stage 0 sporulation protein J

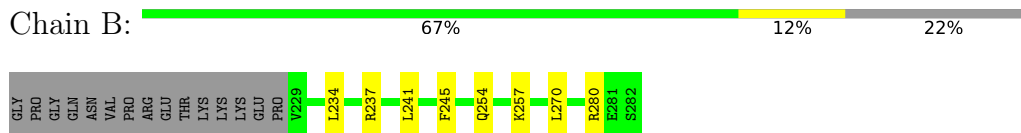


4.2.19 Score per residue for model 19

- Molecule 1: Stage 0 sporulation protein J



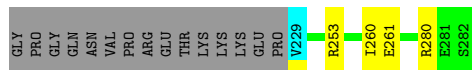
- Molecule 1: Stage 0 sporulation protein J



4.2.20 Score per residue for model 20

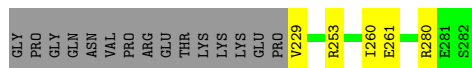
- Molecule 1: Stage 0 sporulation protein J

Chain A:  71% 6% 22%



- Molecule 1: Stage 0 sporulation protein J

Chain B:  71% 7% 22%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	

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	911
Number of shifts mapped to atoms	731
Number of unparsed shifts	0
Number of shifts with mapping errors	180
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	448	455	455	6±3
1	B	455	464	463	6±3
All	All	18060	18380	18360	192

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:LEU:HD11	1:B:270:LEU:HD21	0.63	1.69	5	9
1:A:270:LEU:HD21	1:B:234:LEU:HG	0.63	1.71	8	3
1:A:237:ARG:O	1:A:241:LEU:HG	0.61	1.95	17	18
1:B:237:ARG:O	1:B:241:LEU:HG	0.61	1.95	17	18
1:A:270:LEU:HD21	1:B:234:LEU:HD11	0.61	1.70	2	9
1:A:234:LEU:HG	1:B:270:LEU:HD21	0.61	1.71	8	3
1:B:269:ASP:O	1:B:273:ILE:HG12	0.58	1.99	4	1
1:B:245:PHE:CE1	1:B:276:LEU:HG	0.57	2.34	15	3
1:A:269:ASP:O	1:A:273:ILE:HG12	0.57	1.99	4	1
1:A:245:PHE:CE1	1:A:276:LEU:HG	0.57	2.34	15	3
1:A:261:GLU:HA	1:B:260:ILE:O	0.57	1.99	9	7
1:A:260:ILE:O	1:B:261:GLU:HA	0.56	2.00	9	7
1:A:245:PHE:CD1	1:A:276:LEU:HG	0.56	2.36	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:266:SER:HB3	1:A:269:ASP:OD2	0.55	2.02	15	1
1:B:245:PHE:CD1	1:B:276:LEU:HG	0.55	2.36	4	2
1:A:251:ILE:HB	1:A:253:ARG:NH1	0.54	2.18	17	1
1:B:266:SER:HB3	1:B:269:ASP:OD2	0.53	2.02	15	1
1:B:251:ILE:HB	1:B:253:ARG:NH1	0.53	2.18	17	1
1:A:271:ASP:O	1:A:275:GLU:HG2	0.53	2.03	2	2
1:B:271:ASP:O	1:B:275:GLU:HG2	0.53	2.03	2	2
1:A:264:PHE:CE1	1:A:270:LEU:HD13	0.52	2.39	8	4
1:B:252:LYS:O	1:B:258:GLY:HA3	0.52	2.05	8	4
1:B:264:PHE:CE1	1:B:270:LEU:HD13	0.52	2.39	8	4
1:A:252:LYS:O	1:A:258:GLY:HA3	0.51	2.05	8	5
1:A:264:PHE:CE2	1:A:270:LEU:HD13	0.50	2.41	4	1
1:B:264:PHE:CE2	1:B:270:LEU:HD13	0.50	2.41	4	1
1:B:229:VAL:HG11	1:B:253:ARG:NH2	0.50	2.21	9	2
1:A:278:SER:O	1:A:280:ARG:HG3	0.49	2.07	16	1
1:A:234:LEU:HG	1:B:270:LEU:CD2	0.49	2.38	1	2
1:A:259:LYS:HA	1:B:262:ILE:O	0.49	2.08	13	8
1:A:262:ILE:O	1:B:259:LYS:HA	0.48	2.07	13	5
1:A:270:LEU:HD22	1:B:253:ARG:NH1	0.48	2.23	7	2
1:A:271:ASP:O	1:A:275:GLU:HG3	0.48	2.09	18	3
1:B:271:ASP:O	1:B:275:GLU:HG3	0.48	2.09	18	3
1:A:270:LEU:CD2	1:B:234:LEU:HG	0.48	2.39	1	2
1:B:278:SER:O	1:B:280:ARG:HG3	0.48	2.09	16	1
1:B:270:LEU:O	1:B:274:LEU:HD13	0.47	2.09	17	5
1:A:270:LEU:O	1:A:274:LEU:HD13	0.47	2.10	17	6
1:A:264:PHE:CZ	1:A:270:LEU:HD13	0.47	2.45	17	6
1:B:269:ASP:HA	1:B:272:ARG:NH1	0.46	2.26	6	1
1:B:264:PHE:CZ	1:B:270:LEU:HD13	0.46	2.46	3	6
1:A:253:ARG:NH1	1:B:270:LEU:HD22	0.45	2.26	14	2
1:B:254:GLN:HB2	1:B:257:LYS:O	0.44	2.12	19	2
1:B:266:SER:HB2	1:B:269:ASP:OD1	0.44	2.13	3	1
1:A:279:GLU:HG3	1:B:279:GLU:HG3	0.44	1.90	4	3
1:A:269:ASP:HA	1:A:272:ARG:NH1	0.43	2.27	6	1
1:B:270:LEU:HD12	1:B:274:LEU:HD13	0.43	1.90	9	1
1:A:253:ARG:NH1	1:B:264:PHE:HE1	0.43	2.11	15	1
1:A:266:SER:HB2	1:A:269:ASP:OD1	0.43	2.14	3	1
1:A:254:GLN:HB2	1:A:257:LYS:O	0.43	2.13	19	2
1:A:264:PHE:HE1	1:B:253:ARG:NH1	0.42	2.13	15	1
1:A:260:ILE:HG12	1:B:274:LEU:HD11	0.42	1.92	1	1
1:A:270:LEU:HD12	1:A:274:LEU:HD13	0.42	1.90	9	1
1:B:238:GLU:OE2	1:B:250:ASN:HA	0.42	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:267:ASN:O	1:A:270:LEU:HB3	0.41	2.16	9	1
1:A:274:LEU:HD11	1:B:260:ILE:HG12	0.41	1.91	1	1
1:A:234:LEU:HD11	1:B:270:LEU:CD2	0.41	2.43	5	1
1:A:238:GLU:O	1:A:242:GLN:HG3	0.40	2.15	4	1
1:A:255:LYS:O	1:A:256:LYS:HB2	0.40	2.16	3	1
1:B:267:ASN:O	1:B:270:LEU:HB3	0.40	2.16	9	1
1:B:238:GLU:O	1:B:242:GLN:HG3	0.40	2.16	4	1
1:A:238:GLU:OE2	1:A:250:ASN:HA	0.40	2.17	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	52/69 (75%)	48±1 (93±2%)	3±1 (7±2%)	0±0 (0±1%)	44	80
1	B	52/69 (75%)	48±1 (93±2%)	3±1 (7±2%)	0±0 (0±1%)	44	80
All	All	2080/2760 (75%)	1937 (93%)	137 (7%)	6 (0%)	44	80

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	255	LYS	2
1	B	255	LYS	2
1	A	279	GLU	1
1	B	279	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/64 (78%)	48±1 (96±2%)	2±1 (4±2%)	36	84
1	B	51/64 (80%)	49±1 (96±2%)	2±1 (4±2%)	37	85
All	All	2020/2560 (79%)	1944 (96%)	76 (4%)	36	84

All 14 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	280	ARG	15
1	B	280	ARG	15
1	A	245	PHE	14
1	B	245	PHE	14
1	A	272	ARG	4
1	B	272	ARG	4
1	A	253	ARG	2
1	B	253	ARG	2
1	A	259	LYS	1
1	B	259	LYS	1
1	A	269	ASP	1
1	B	269	ASP	1
1	A	279	GLU	1
1	B	279	GLU	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 monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping i

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	911
Number of shifts mapped to atoms	731
Number of unparsed shifts	0
Number of shifts with mapping errors	180
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 180 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	215	PRO	CG	27.092	0.055	1
1	A	215	PRO	CD	49.673	0.036	1
1	A	215	PRO	CA	63.529	0.120	1
1	A	215	PRO	C	177.449	0.000	1
1	A	215	PRO	CB	32.36	0.147	1
1	A	215	PRO	HA	4.47	0.007	1
1	A	215	PRO	HB2	1.984	0.000	2
1	A	215	PRO	HB3	2.301	0.002	2
1	A	215	PRO	HG2	2.029	0.000	1
1	A	215	PRO	HG3	2.029	0.000	1
1	A	215	PRO	HD2	3.57	0.000	2
1	A	215	PRO	HD3	3.595	0.000	2
1	A	216	GLY	C	174.074	0.000	1
1	A	216	GLY	CA	45.349	0.012	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	216	GLY	H	8.567	0.001	1
1	A	216	GLY	HA2	3.954	0.000	1
1	A	216	GLY	HA3	3.954	0.000	1
1	A	216	GLY	N	109.785	0.008	1
1	A	217	GLN	CA	55.885	0.059	1
1	A	217	GLN	C	175.705	0.000	1
1	A	217	GLN	CB	29.742	0.106	1
1	A	217	GLN	CG	33.947	0.135	1
1	A	217	GLN	CD	180.587	0.015	1
1	A	217	GLN	H	8.115	0.001	1
1	A	217	GLN	HE21	6.818	0.001	1
1	A	217	GLN	HE22	7.482	0.001	1
1	A	217	GLN	HA	4.358	0.003	1
1	A	217	GLN	HG2	2.328	0.003	2
1	A	217	GLN	HG3	2.328	0.003	2
1	A	217	GLN	HB2	1.985	0.002	2
1	A	217	GLN	HB3	2.091	0.002	2
1	A	217	GLN	N	119.371	0.005	1
1	A	217	GLN	NE2	111.992	0.215	1
1	A	218	ASN	C	174.656	0.000	1
1	A	218	ASN	CB	38.882	0.027	1
1	A	218	ASN	CA	53.355	0.074	1
1	A	218	ASN	CG	177.134	0.007	1
1	A	218	ASN	HD21	6.871	0.002	1
1	A	218	ASN	HD22	7.527	0.022	1
1	A	218	ASN	H	8.498	0.001	1
1	A	218	ASN	HA	4.707	0.004	1
1	A	218	ASN	HB2	2.726	0.006	2
1	A	218	ASN	HB3	2.796	0.007	2
1	A	218	ASN	ND2	112.955	0.145	1
1	A	218	ASN	N	120.188	0.010	1
1	A	219	VAL	CB	32.61	0.059	1
1	A	219	VAL	CA	59.87	0.139	1
1	A	219	VAL	CG1	20.391	0.000	1
1	A	219	VAL	CG2	20.391	0.000	1
1	A	219	VAL	H	7.987	0.001	1
1	A	219	VAL	HA	4.41	0.003	1
1	A	219	VAL	HB	2.065	0.001	1
1	A	219	VAL	HG11	0.911	0.011	2
1	A	219	VAL	HG12	0.911	0.011	2
1	A	219	VAL	HG13	0.911	0.011	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	219	VAL	HG21	0.942	0.012	2
1	A	219	VAL	HG22	0.942	0.012	2
1	A	219	VAL	HG23	0.942	0.012	2
1	A	219	VAL	N	121.592	0.016	1
1	A	220	PRO	CG	24.858	0.000	1
1	A	220	PRO	CD	50.203	0.000	1
1	A	220	PRO	C	176.051	0.000	1
1	A	220	PRO	CA	62.78	0.015	1
1	A	220	PRO	CB	34.487	0.007	1
1	A	220	PRO	HA	4.712	0.000	1
1	A	220	PRO	HD2	3.545	0.000	1
1	A	220	PRO	HD3	3.545	0.000	1
1	A	220	PRO	HG2	1.859	0.000	2
1	A	220	PRO	HB2	2.106	0.000	2
1	A	220	PRO	HB3	2.379	0.000	2
1	A	220	PRO	HG3	1.928	0.000	2
1	A	221	ARG	CB	30.93	0.056	1
1	A	221	ARG	CA	56.468	0.145	1
1	A	221	ARG	CG	27.137	0.000	1
1	A	221	ARG	CD	43.434	0.000	1
1	A	221	ARG	C	176.357	0.000	1
1	A	221	ARG	H	8.536	0.002	1
1	A	221	ARG	HD2	3.209	0.000	1
1	A	221	ARG	HD3	3.209	0.000	1
1	A	221	ARG	HA	4.303	0.002	1
1	A	221	ARG	HB2	1.802	0.000	1
1	A	221	ARG	HB3	1.802	0.000	1
1	A	221	ARG	HG2	1.673	0.000	1
1	A	221	ARG	HG3	1.673	0.000	1
1	A	221	ARG	N	121.447	0.022	1
1	A	222	GLU	CB	30.556	0.064	1
1	A	222	GLU	CG	36.259	0.000	1
1	A	222	GLU	C	176.536	0.000	1
1	A	222	GLU	CA	56.497	0.055	1
1	A	222	GLU	H	8.444	0.001	1
1	A	222	GLU	HB2	1.95	0.000	2
1	A	222	GLU	HB3	2.037	0.000	2
1	A	222	GLU	HG2	2.242	0.000	1
1	A	222	GLU	HG3	2.242	0.000	1
1	A	222	GLU	HA	4.364	0.000	1
1	A	222	GLU	N	122.061	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	THR	C	174.443	0.000	1
1	A	223	THR	CB	69.854	0.062	1
1	A	223	THR	CA	61.995	0.055	1
1	A	223	THR	CG2	21.818	0.000	1
1	A	223	THR	H	8.232	0.001	1
1	A	223	THR	HB	4.19	0.000	1
1	A	223	THR	HG23	1.193	0.000	1
1	A	223	THR	HG22	1.193	0.000	1
1	A	223	THR	HG21	1.193	0.000	1
1	A	223	THR	HA	4.316	0.000	1
1	A	223	THR	N	116.334	0.007	1
1	A	224	LYS	CE	42.246	0.000	1
1	A	224	LYS	CG	24.662	0.000	1
1	A	224	LYS	CD	28.974	0.000	1
1	A	224	LYS	C	176.303	0.000	1
1	A	224	LYS	CA	56.29	0.055	1
1	A	224	LYS	CB	33.124	0.043	1
1	A	224	LYS	H	8.284	0.001	1
1	A	224	LYS	HA	4.331	0.000	1
1	A	224	LYS	HG2	1.426	0.000	1
1	A	224	LYS	HG3	1.426	0.000	1
1	A	224	LYS	HE2	2.997	0.000	1
1	A	224	LYS	HE3	2.997	0.000	1
1	A	224	LYS	HB2	1.748	0.000	2
1	A	224	LYS	HB3	1.815	0.000	2
1	A	224	LYS	HD2	1.685	0.000	1
1	A	224	LYS	HD3	1.685	0.000	1
1	A	224	LYS	N	124.115	0.021	1
1	A	225	LYS	CB	33.148	0.000	1
1	A	225	LYS	CG	24.709	0.000	1
1	A	225	LYS	CD	28.967	0.000	1
1	A	225	LYS	CE	42.265	0.000	1
1	A	225	LYS	C	176.276	0.000	1
1	A	225	LYS	CA	56.297	0.057	1
1	A	225	LYS	HE3	2.999	0.000	1
1	A	225	LYS	HG2	1.427	0.000	1
1	A	225	LYS	HG3	1.427	0.000	1
1	A	225	LYS	HD2	1.674	0.000	1
1	A	225	LYS	H	8.3	0.001	1
1	A	225	LYS	HD3	1.674	0.000	1
1	A	225	LYS	HB2	1.738	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	LYS	HB3	1.806	0.000	2
1	A	225	LYS	HA	4.292	0.000	1
1	A	225	LYS	HE2	2.999	0.000	1
1	A	225	LYS	N	123.31	0.013	1
1	A	226	LYS	CB	33.183	0.015	1
1	A	226	LYS	CG	24.708	0.000	1
1	A	226	LYS	CD	29.029	0.000	1
1	A	226	LYS	CE	42.264	0.000	1
1	A	226	LYS	C	176.19	0.000	1
1	A	226	LYS	CA	56.184	0.072	1
1	A	226	LYS	H	8.353	0.005	1
1	A	226	LYS	HA	4.311	0.000	1
1	A	226	LYS	HE2	2.999	0.000	1
1	A	226	LYS	HE3	2.999	0.000	1
1	A	226	LYS	HG2	1.427	0.000	1
1	A	226	LYS	HG3	1.427	0.000	1
1	A	226	LYS	HB2	1.723	0.000	2
1	A	226	LYS	HD2	1.723	0.000	1
1	A	226	LYS	HD3	1.723	0.000	1
1	A	226	LYS	HB3	1.796	0.000	2
1	A	226	LYS	N	123.509	0.033	1
1	A	227	GLU	CB	29.949	0.000	1
1	A	227	GLU	CA	54.447	0.065	1
1	A	227	GLU	CG	36.128	0.000	1
1	A	227	GLU	H	8.368	0.002	1
1	A	227	GLU	HB2	1.879	0.000	2
1	A	227	GLU	HB3	2.032	0.000	2
1	A	227	GLU	HG2	2.287	0.000	2
1	A	227	GLU	HG3	2.283	0.000	2
1	A	227	GLU	HA	4.582	0.000	1
1	A	227	GLU	N	124.084	0.018	1
1	A	228	PRO	CA	62.868	0.007	1
1	A	228	PRO	CB	32.169	0.009	1
1	A	228	PRO	C	176.903	0.000	1
1	A	228	PRO	CG	27.493	0.000	1
1	A	228	PRO	CD	50.694	0.000	1
1	A	228	PRO	HA	4.453	0.000	1
1	A	228	PRO	HD2	3.697	0.000	2
1	A	228	PRO	HD3	3.813	0.000	2
1	A	228	PRO	HG2	2.034	0.000	1
1	A	228	PRO	HG3	2.034	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	228	PRO	HB2	1.858	0.000	2
1	A	228	PRO	HB3	2.266	0.000	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	68	-0.56 ± 0.13	Should be checked
$^{13}\text{C}_\beta$	65	0.09 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	64	-0.11 ± 0.13	None needed (< 0.5 ppm)
^{15}N	64	-0.04 ± 0.26	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 716 atoms were assigned a chemical shift out of a possible 1575. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	262/539 (49%)	106/218 (49%)	104/214 (49%)	52/107 (49%)
Sidechain	416/940 (44%)	278/597 (47%)	129/295 (44%)	9/48 (19%)
Aromatic	38/96 (40%)	19/46 (41%)	19/50 (38%)	0/0 (—%)
Overall	716/1575 (45%)	403/861 (47%)	252/559 (45%)	61/155 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 731 atoms were assigned a chemical shift out of a possible 1590. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	267/544 (49%)	108/220 (49%)	106/216 (49%)	53/108 (49%)
Sidechain	426/950 (45%)	285/604 (47%)	132/298 (44%)	9/48 (19%)
Aromatic	38/96 (40%)	19/46 (41%)	19/50 (38%)	0/0 (—%)
Overall	731/1590 (46%)	412/870 (47%)	257/564 (46%)	62/156 (40%)

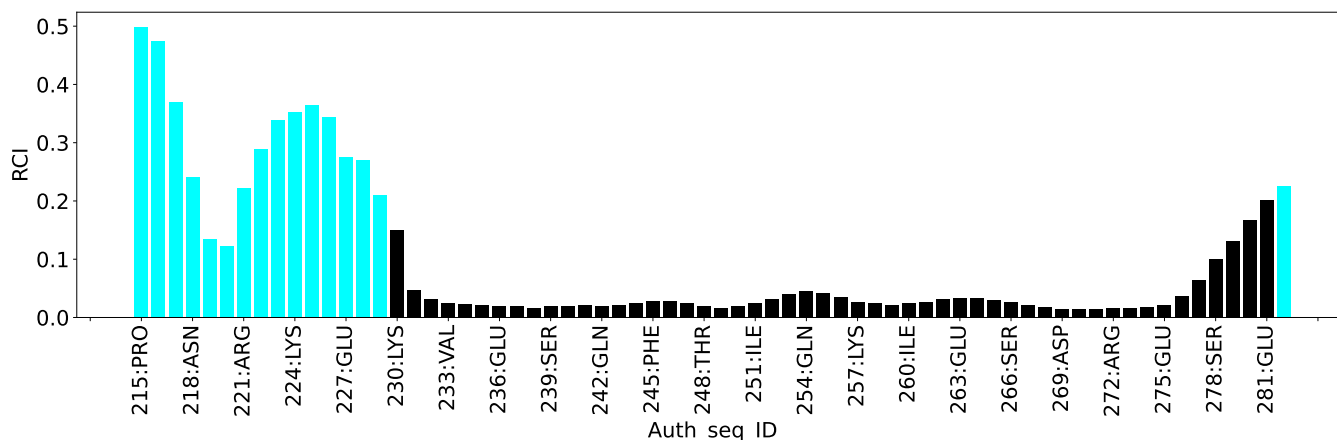
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	4044
Intra-residue ($ i-j =0$)	1080
Sequential ($ i-j =1$)	790
Medium range ($ i-j >1$ and $ i-j <5$)	962
Long range ($ i-j \geq 5$)	724
Inter-chain	438
Hydrogen bond restraints	50
Disulfide bond restraints	0
Total dihedral-angle restraints	160
Number of unmapped restraints	0
Number of restraints per residue	30.5
Number of long range restraints per residue ¹	5.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	30.2	0.2
0.2-0.5 (Medium)	45.6	0.5
>0.5 (Large)	52.7	2.46

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)	1.4	2.8
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

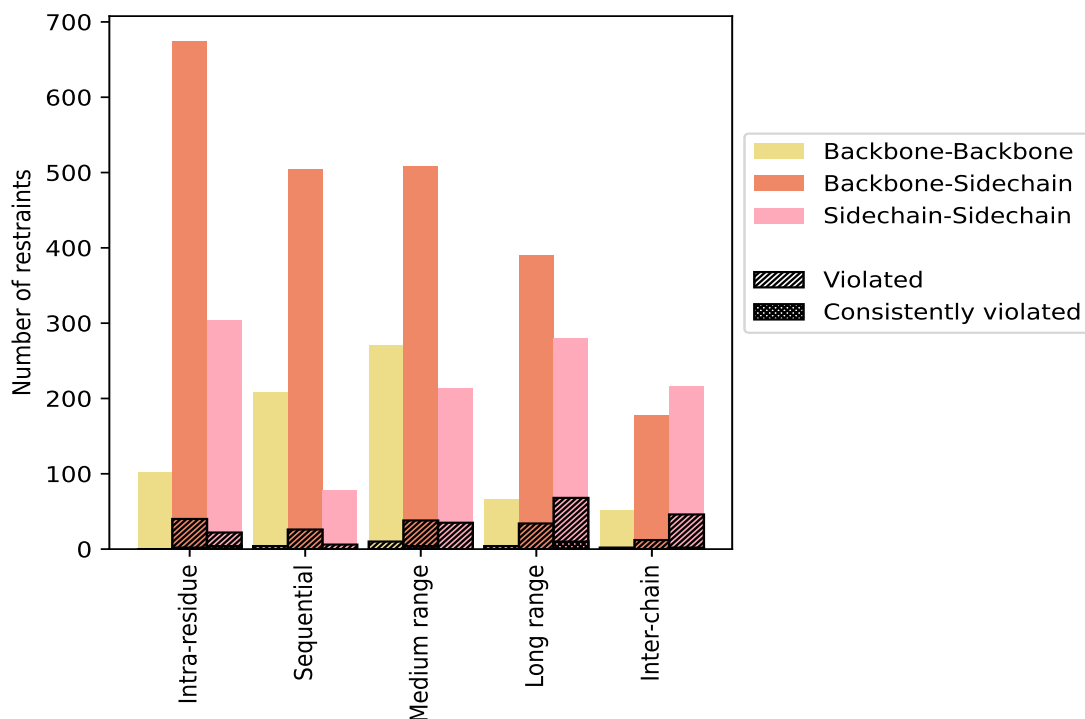
9.1 Summary of distance violations [i](#)

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 ($i-j =0$)	1080	26.7	62	5.7	1.5	6	0.6	0.1
Backbone-Backbone	102	2.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	674	16.7	40	5.9	1.0	2	0.3	0.0
Sidechain-Sidechain	304	7.5	22	7.2	0.5	4	1.3	0.1
Sequential ($i-j =1$)	790	19.5	36	4.6	0.9	0	0.0	0.0
Backbone-Backbone	208	5.1	4	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	504	12.5	26	5.2	0.6	0	0.0	0.0
Sidechain-Sidechain	78	1.9	6	7.7	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	962	23.8	75	7.8	1.9	4	0.4	0.1
Backbone-Backbone	240	5.9	2	0.8	0.0	0	0.0	0.0
Backbone-Sidechain	508	12.6	38	7.5	0.9	4	0.8	0.1
Sidechain-Sidechain	214	5.3	35	16.4	0.9	0	0.0	0.0
Long range ($i-j \geq 5$)	724	17.9	106	14.6	2.6	10	1.4	0.2
Backbone-Backbone	54	1.3	4	7.4	0.1	0	0.0	0.0
Backbone-Sidechain	390	9.6	34	8.7	0.8	0	0.0	0.0
Sidechain-Sidechain	280	6.9	68	24.3	1.7	10	3.6	0.2
Inter-chain	438	10.8	60	13.7	1.5	2	0.5	0.0
Backbone-Backbone	44	1.1	2	4.5	0.0	0	0.0	0.0
Backbone-Sidechain	178	4.4	12	6.7	0.3	0	0.0	0.0
Sidechain-Sidechain	216	5.3	46	21.3	1.1	2	0.9	0.0
Hydrogen bond	50	1.2	8	16.0	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4044	100.0	347	8.6	8.6	22	0.5	0.5
Backbone-Backbone	698	17.3	20	2.9	0.5	0	0.0	0.0
Backbone-Sidechain	2254	55.7	150	6.7	3.7	6	0.3	0.1
Sidechain-Sidechain	1092	27.0	177	16.2	4.4	16	1.5	0.4

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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	22	10	27	46	22	127	0.62	2.46	0.51	0.47
2	26	12	20	30	24	112	0.62	2.42	0.58	0.46
3	28	8	36	46	23	141	0.53	2.29	0.42	0.4
4	28	8	24	31	20	111	0.6	2.24	0.48	0.51
5	28	14	23	40	23	128	0.5	2.22	0.4	0.38
6	26	14	36	32	26	134	0.55	2.27	0.46	0.42
7	30	14	28	36	21	129	0.59	2.41	0.54	0.38
8	26	12	24	56	32	150	0.58	2.21	0.45	0.43
9	27	12	22	42	26	129	0.56	2.21	0.43	0.44
10	23	14	30	38	26	131	0.5	1.98	0.36	0.45
11	32	14	40	42	22	150	0.56	2.09	0.5	0.36

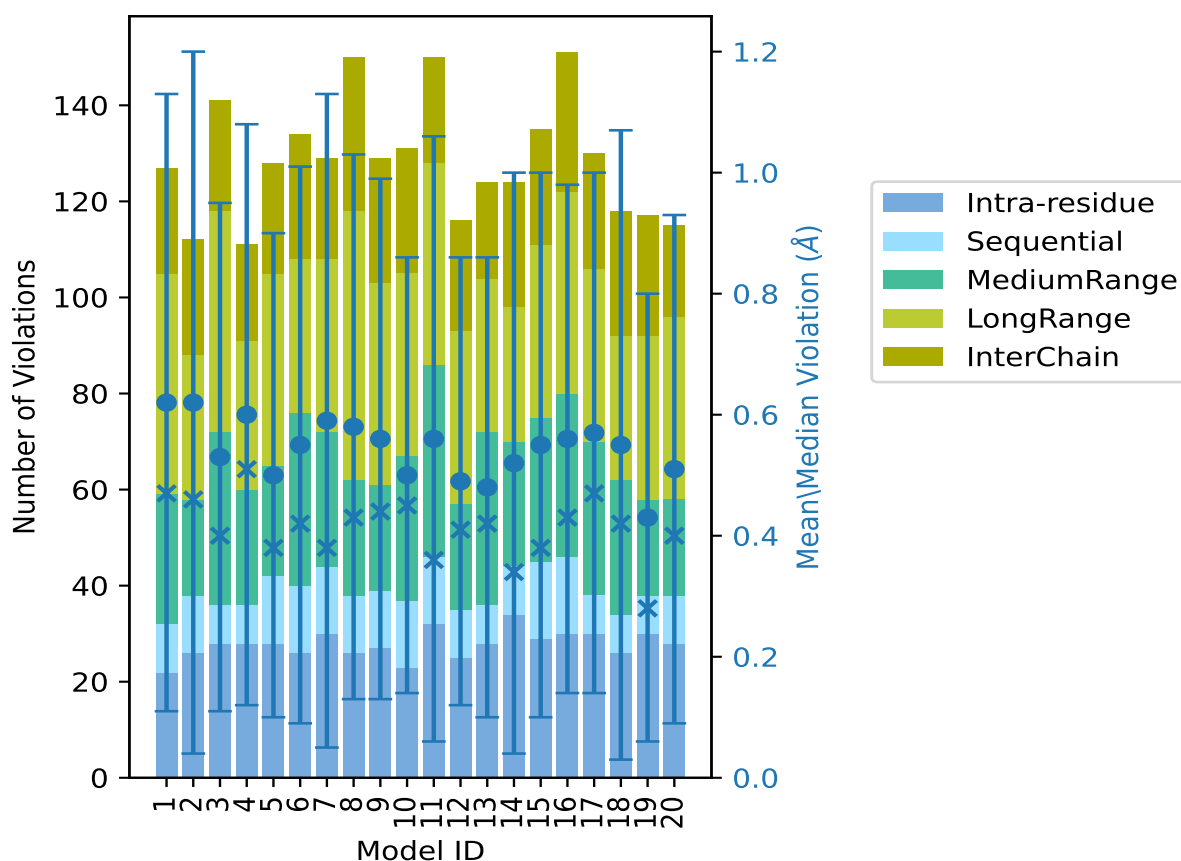
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	25	10	22	36	23	116	0.49	1.87	0.37	0.41
13	28	8	36	32	20	124	0.48	2.29	0.38	0.42
14	34	10	26	28	26	124	0.52	2.29	0.48	0.34
15	29	16	30	36	24	135	0.55	2.21	0.45	0.38
16	30	16	34	42	29	151	0.56	2.35	0.42	0.43
17	30	8	32	36	24	130	0.57	2.24	0.43	0.47
18	26	8	28	30	26	118	0.55	2.4	0.52	0.42
19	30	8	20	34	25	117	0.43	2.12	0.37	0.28
20	28	10	20	38	19	115	0.51	2.05	0.42	0.4

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

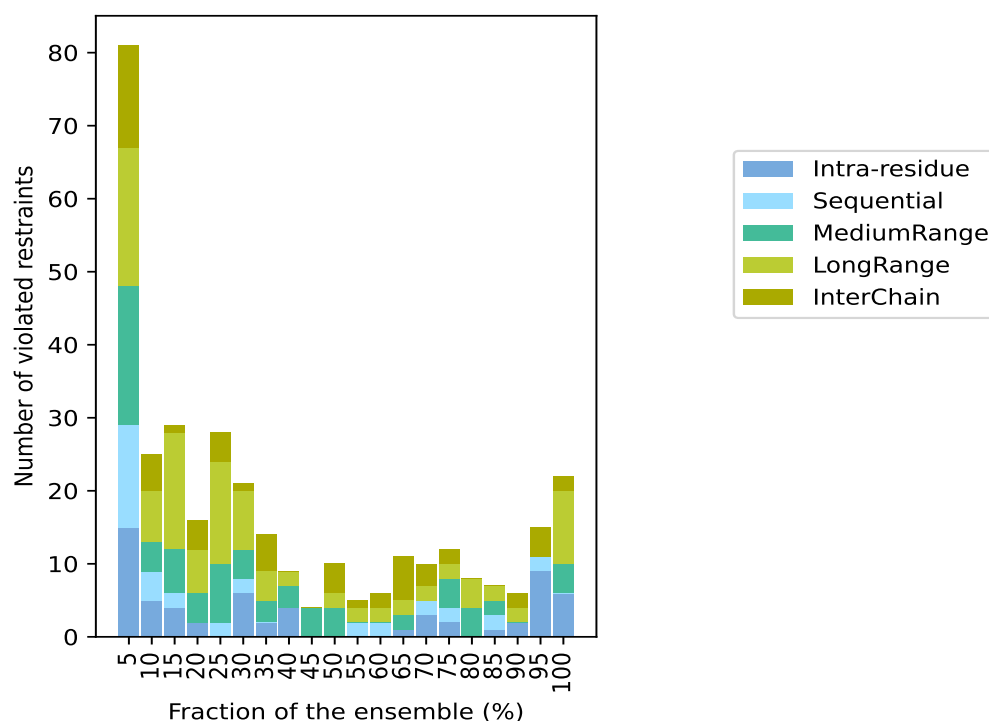
9.3 Distance violation statistics for the ensemble

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, 3655(IR:1018, SQ:754, MR:887, LR:618, IC:378) 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	%
15	14	19	19	14	81	1	5.0
5	4	4	7	5	25	2	10.0
4	2	6	16	1	29	3	15.0
2	0	4	6	4	16	4	20.0
0	2	8	14	4	28	5	25.0
6	2	4	8	1	21	6	30.0
2	0	3	4	5	14	7	35.0
4	0	3	2	0	9	8	40.0
0	0	4	0	0	4	9	45.0
0	0	4	2	4	10	10	50.0
0	2	0	2	1	5	11	55.0
0	2	0	2	2	6	12	60.0
1	0	2	2	6	11	13	65.0
3	2	0	2	3	10	14	70.0
2	2	4	2	2	12	15	75.0
0	0	4	4	0	8	16	80.0
1	2	2	2	0	7	17	85.0
2	0	0	2	2	6	18	90.0
9	2	0	0	4	15	19	95.0
6	0	4	10	2	22	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

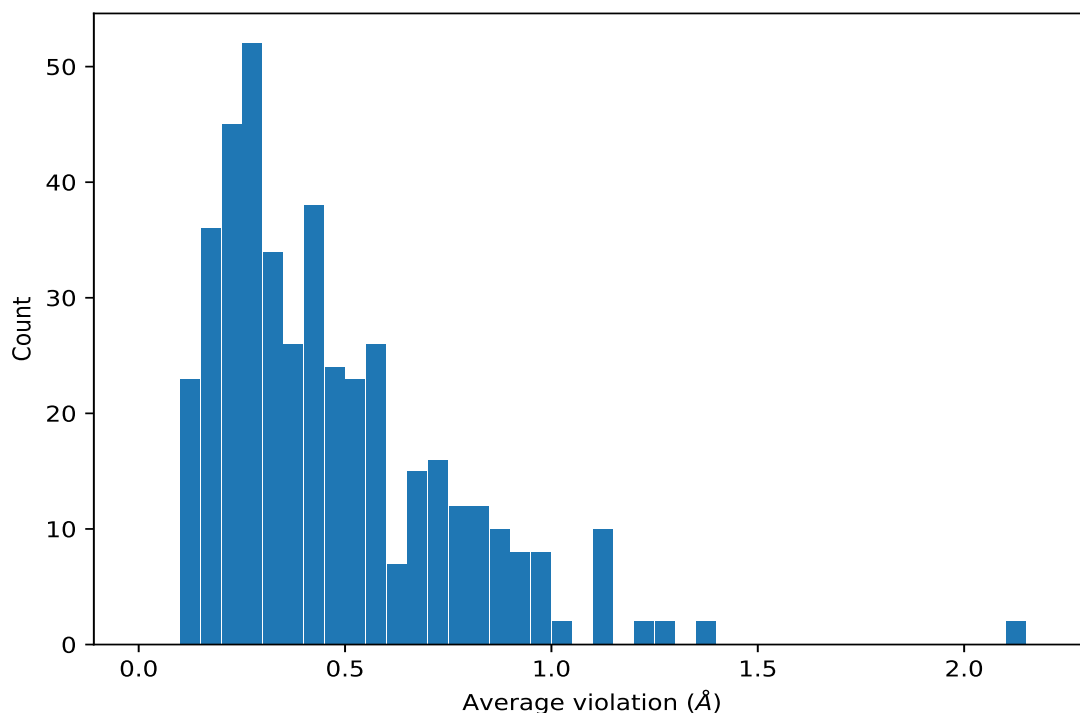
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	20	2.13	0.15	2.17
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	20	2.13	0.15	2.17
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	20	1.36	0.42	1.5
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	20	1.36	0.42	1.5
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	20	1.14	0.42	1.14
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	20	1.14	0.42	1.14
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	20	1.12	0.52	1.06
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	20	1.12	0.52	1.06
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	20	0.93	0.17	0.86
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	20	0.93	0.17	0.87
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	20	0.92	0.77	0.6
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	20	0.91	0.77	0.59
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	20	0.5	0.14	0.5
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	20	0.5	0.1	0.52
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	20	0.5	0.1	0.52
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	20	0.5	0.14	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	20	0.5	0.1	0.52
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	20	0.5	0.1	0.52
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	20	0.46	0.02	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	20	0.46	0.02	0.46
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	20	0.37	0.12	0.38
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	20	0.36	0.12	0.38
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	20	0.17	0.01	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	20	0.17	0.01	0.17
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	19	0.8	0.07	0.77
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	19	0.8	0.08	0.77
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	19	0.63	0.33	0.56
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	19	0.62	0.33	0.54
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	19	0.45	0.19	0.39
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	19	0.45	0.19	0.39
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	19	0.44	0.06	0.43
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	19	0.44	0.06	0.42
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	19	0.4	0.3	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	19	0.4	0.3	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	19	0.4	0.3	0.31
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	19	0.4	0.3	0.3
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	19	0.4	0.3	0.3
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	19	0.4	0.3	0.3
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	19	0.17	0.01	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	19	0.17	0.01	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	19	0.17	0.01	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	19	0.17	0.01	0.17
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	19	0.13	0.01	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	19	0.13	0.01	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	19	0.12	0.01	0.13
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	18	0.76	0.2	0.7
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	18	0.76	0.2	0.7
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	18	0.76	0.2	0.7
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	18	0.76	0.2	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	18	0.76	0.2	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	18	0.76	0.2	0.69
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	18	0.53	0.24	0.58
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	18	0.53	0.24	0.58
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	18	0.53	0.24	0.58
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	18	0.53	0.24	0.58
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	18	0.53	0.24	0.58
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	18	0.53	0.24	0.58
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	18	0.39	0.23	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	18	0.39	0.23	0.3
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	17	0.37	0.17	0.29
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	17	0.37	0.17	0.29
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	17	0.25	0.08	0.24
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	17	0.25	0.08	0.24
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	17	0.25	0.08	0.24
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	17	0.25	0.08	0.24
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	17	0.25	0.08	0.24
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	17	0.25	0.08	0.24
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	17	0.21	0.05	0.22
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	17	0.21	0.05	0.22
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	17	0.13	0.01	0.13
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	16	0.69	0.74	0.32
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	16	0.69	0.74	0.32
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	16	0.69	0.74	0.32
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	16	0.69	0.74	0.32
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	16	0.69	0.74	0.32
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	16	0.69	0.74	0.32
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	16	0.58	0.17	0.61
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	16	0.58	0.17	0.62
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	16	0.51	0.24	0.54
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	16	0.5	0.24	0.53
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	16	0.26	0.05	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	16	0.26	0.05	0.27
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	16	0.26	0.05	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	16	0.26	0.05	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	16	0.26	0.05	0.27
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	16	0.26	0.05	0.27
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	15	0.97	0.91	0.34
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	15	0.97	0.91	0.34
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	15	0.74	0.17	0.75
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	15	0.74	0.17	0.75
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	15	0.74	0.17	0.75
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	15	0.74	0.17	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	15	0.74	0.17	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	15	0.74	0.17	0.74
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	15	0.72	0.14	0.71
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	15	0.72	0.14	0.72
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	15	0.49	0.5	0.21
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	15	0.49	0.5	0.21
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	15	0.48	0.19	0.49
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	15	0.48	0.18	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	15	0.45	0.37	0.21
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	15	0.45	0.37	0.21
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	14	0.63	0.1	0.62
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	14	0.63	0.1	0.63
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	14	0.54	0.0	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	14	0.54	0.0	0.54
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	14	0.35	0.21	0.28
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	14	0.34	0.09	0.32
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	14	0.34	0.09	0.32
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	14	0.34	0.09	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	14	0.34	0.09	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	14	0.34	0.09	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	14	0.34	0.09	0.32
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	14	0.2	0.03	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	14	0.2	0.03	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	14	0.2	0.03	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	14	0.19	0.03	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	14	0.19	0.03	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	14	0.19	0.03	0.2
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	14	0.13	0.02	0.13
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	13	0.83	0.46	0.78
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	13	0.82	0.47	0.82
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	13	0.76	0.41	0.85
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	13	0.76	0.41	0.85
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	13	0.76	0.41	0.85
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	13	0.76	0.41	0.85
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	13	0.55	0.07	0.58
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	13	0.55	0.08	0.56
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	13	0.41	0.37	0.24
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	13	0.36	0.22	0.28
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	13	0.28	0.09	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	13	0.28	0.09	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	13	0.28	0.09	0.29
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	13	0.28	0.09	0.29
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	13	0.28	0.08	0.28
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	13	0.28	0.08	0.28
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	13	0.28	0.08	0.28
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	13	0.28	0.08	0.28
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	13	0.14	0.02	0.14
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	12	1.02	0.2	0.94
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	12	1.02	0.2	0.94
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	12	0.45	0.23	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	12	0.45	0.24	0.37
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	12	0.39	0.24	0.34
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	12	0.39	0.24	0.34
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	12	0.39	0.24	0.34
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	12	0.39	0.24	0.34
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	12	0.28	0.13	0.24
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	12	0.27	0.13	0.24
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	11	1.22	0.66	1.27
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	11	1.22	0.66	1.26
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	11	0.46	0.39	0.3
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	11	0.24	0.08	0.22
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	11	0.24	0.08	0.22
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	11	0.24	0.08	0.22
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	11	0.24	0.08	0.22
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	10	0.85	0.48	0.94
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	10	0.85	0.48	0.94
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	10	0.44	0.19	0.46
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	10	0.42	0.21	0.4
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	10	0.38	0.2	0.34
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	10	0.38	0.3	0.29
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	10	0.38	0.2	0.34
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	10	0.37	0.3	0.29
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	10	0.27	0.08	0.28
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	10	0.26	0.07	0.28
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	9	0.88	0.5	1.04
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	9	0.88	0.5	1.04
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	9	0.44	0.45	0.33
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	9	0.44	0.45	0.33
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	9	0.44	0.45	0.32
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	9	0.44	0.45	0.32
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	8	0.6	0.01	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	8	0.6	0.01	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	8	0.6	0.01	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	8	0.6	0.01	0.6
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	8	0.55	0.41	0.42
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	8	0.55	0.41	0.42
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	8	0.55	0.4	0.42
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	8	0.55	0.4	0.42
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	8	0.46	0.27	0.46
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	8	0.27	0.0	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	8	0.27	0.0	0.27
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	8	0.26	0.09	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	8	0.26	0.09	0.28
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	7	0.97	0.55	1.04
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	7	0.97	0.55	1.04
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	7	0.97	0.55	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	7	0.96	0.54	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	7	0.96	0.54	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	7	0.96	0.54	1.04
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	7	0.83	0.2	0.9
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	7	0.82	0.2	0.9
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	7	0.65	0.69	0.24
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	7	0.63	0.69	0.21
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	7	0.52	0.25	0.59
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	7	0.39	0.22	0.36
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	7	0.39	0.21	0.36
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	7	0.39	0.21	0.36
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	7	0.36	0.16	0.33
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	7	0.35	0.15	0.34
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	7	0.35	0.2	0.29
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	7	0.35	0.19	0.31
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	7	0.33	0.14	0.33
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	7	0.32	0.14	0.33
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	6	0.74	0.18	0.77
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	6	0.74	0.18	0.77
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	6	0.68	0.12	0.7
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	6	0.68	0.12	0.7
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	6	0.56	0.03	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	6	0.56	0.03	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	6	0.56	0.03	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	6	0.56	0.03	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	6	0.56	0.03	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	6	0.56	0.03	0.56
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	6	0.54	0.58	0.14
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	6	0.54	0.58	0.14
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	6	0.54	0.11	0.55
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	6	0.53	0.11	0.55
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	6	0.47	0.21	0.5
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	6	0.47	0.21	0.5
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	6	0.47	0.21	0.5
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	6	0.47	0.21	0.5
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	6	0.47	0.21	0.5
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	6	0.47	0.21	0.5
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	6	0.45	0.21	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	6	0.41	0.09	0.43
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	6	0.4	0.09	0.43
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	6	0.39	0.19	0.38
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	6	0.39	0.19	0.38
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	6	0.39	0.2	0.38
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	6	0.39	0.2	0.38
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	6	0.26	0.07	0.26
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	6	0.26	0.07	0.26
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	6	0.26	0.07	0.26
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	6	0.26	0.07	0.26
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	6	0.26	0.07	0.26
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	6	0.26	0.07	0.26
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	6	0.14	0.0	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	6	0.14	0.0	0.14
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	5	1.12	0.7	0.84
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	5	1.12	0.33	1.24
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	5	1.12	0.33	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	5	1.12	0.33	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	5	1.12	0.33	1.24
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	5	1.12	0.7	0.83
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	5	0.95	0.28	0.99
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	5	0.95	0.28	0.99
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	5	0.87	0.22	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	5	0.87	0.22	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	5	0.87	0.22	1.02
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	5	0.86	0.21	1.01
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	5	0.86	0.21	1.01
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	5	0.86	0.21	1.01
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	5	0.79	0.18	0.79
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	5	0.79	0.18	0.79
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	5	0.72	0.19	0.61
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	5	0.72	0.19	0.61
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	5	0.72	0.19	0.61
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	5	0.72	0.19	0.6
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	5	0.72	0.19	0.6
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	5	0.72	0.19	0.6
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	5	0.63	0.06	0.62
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	5	0.63	0.06	0.62
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	5	0.49	0.34	0.44
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	5	0.49	0.34	0.43
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	5	0.45	0.14	0.39
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	5	0.44	0.14	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	5	0.33	0.12	0.38
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	5	0.33	0.12	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	5	0.33	0.12	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	5	0.33	0.12	0.38
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	5	0.28	0.05	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	5	0.28	0.05	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	5	0.28	0.05	0.3
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	5	0.28	0.05	0.3
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	5	0.28	0.04	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	5	0.28	0.04	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	5	0.28	0.04	0.29
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	5	0.28	0.04	0.29
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	5	0.2	0.03	0.2
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	5	0.2	0.03	0.19
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	5	0.19	0.05	0.18
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	5	0.19	0.05	0.18
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	5	0.19	0.05	0.18
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	5	0.19	0.05	0.18
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	5	0.18	0.05	0.18
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	5	0.18	0.05	0.18
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	5	0.18	0.05	0.18
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	5	0.18	0.05	0.18
(2,26)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	4	0.8	0.51	0.58
(2,25)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	4	0.8	0.52	0.58
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG2	4	0.57	0.03	0.57
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG3	4	0.57	0.03	0.57
(1,3129)	1:A:236:GLU:HG2	1:A:234:LEU:HB2	4	0.57	0.03	0.57
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG2	4	0.56	0.03	0.56
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG3	4	0.56	0.03	0.56
(1,3130)	1:B:236:GLU:HG2	1:B:234:LEU:HB2	4	0.56	0.03	0.56
(1,1190)	1:B:276:LEU:HD11	1:B:245:PHE:HE1	4	0.5	0.21	0.56
(1,1189)	1:A:276:LEU:HD11	1:A:245:PHE:HE1	4	0.5	0.21	0.56
(1,3301)	1:A:232:ALA:HB1	1:A:230:LYS:HB3	4	0.44	0.31	0.39
(1,3301)	1:A:232:ALA:HB1	1:A:235:LYS:HB2	4	0.44	0.31	0.39
(1,3302)	1:B:232:ALA:HB1	1:B:230:LYS:HB3	4	0.43	0.31	0.38
(1,3302)	1:B:232:ALA:HB1	1:B:235:LYS:HB2	4	0.43	0.31	0.38
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD22	4	0.33	0.17	0.28
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD21	4	0.33	0.17	0.28
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD23	4	0.33	0.17	0.28
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD22	4	0.33	0.15	0.28
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD21	4	0.33	0.15	0.28
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD23	4	0.33	0.15	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG21	4	0.28	0.1	0.28
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG22	4	0.28	0.1	0.28
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG23	4	0.28	0.1	0.28
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG21	4	0.28	0.11	0.28
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG22	4	0.28	0.11	0.28
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG23	4	0.28	0.11	0.28
(1,1699)	1:A:243:ASN:HD22	1:A:243:ASN:HB3	4	0.24	0.01	0.24
(1,1700)	1:B:243:ASN:HD22	1:B:243:ASN:HB3	4	0.24	0.0	0.24
(1,1043)	1:A:234:LEU:HB3	1:B:270:LEU:HD11	4	0.15	0.05	0.14
(1,1044)	1:B:234:LEU:HB3	1:A:270:LEU:HD11	4	0.15	0.05	0.12
(3,24)	1:A:279:GLU:H	1:A:275:GLU:O	3	1.26	0.15	1.19
(3,48)	1:B:279:GLU:H	1:B:275:GLU:O	3	1.25	0.15	1.17
(1,375)	1:A:262:ILE:HG21	1:A:245:PHE:HB2	3	0.91	0.08	0.87
(1,376)	1:B:262:ILE:HG21	1:B:245:PHE:HB2	3	0.91	0.08	0.87
(1,1349)	1:A:230:LYS:H	1:A:230:LYS:HB2	3	0.82	0.04	0.81
(1,1350)	1:B:230:LYS:H	1:B:230:LYS:HB2	3	0.81	0.04	0.81
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD12	3	0.65	0.24	0.69
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD11	3	0.65	0.24	0.69
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD13	3	0.65	0.24	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD12	3	0.65	0.24	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD11	3	0.65	0.24	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD13	3	0.65	0.24	0.69
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG22	3	0.4	0.03	0.41
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG21	3	0.4	0.03	0.41
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG23	3	0.4	0.03	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD12	3	0.4	0.03	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD11	3	0.4	0.03	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD13	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG22	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG21	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG23	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD12	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD11	3	0.4	0.03	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD13	3	0.4	0.03	0.41
(1,363)	1:A:262:ILE:HG21	1:A:245:PHE:HB3	3	0.36	0.2	0.25
(1,364)	1:B:262:ILE:HG21	1:B:245:PHE:HB3	3	0.36	0.2	0.25
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD22	3	0.24	0.03	0.23
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD21	3	0.24	0.03	0.23
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD23	3	0.24	0.03	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD22	3	0.24	0.03	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD21	3	0.24	0.03	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD23	3	0.24	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG22	3	0.22	0.12	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG21	3	0.22	0.12	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG23	3	0.22	0.12	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD12	3	0.22	0.12	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD11	3	0.22	0.12	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD13	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG22	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG21	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG23	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD12	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD11	3	0.22	0.12	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD13	3	0.22	0.12	0.17
(1,2351)	1:A:266:SER:H	1:A:264:PHE:HD2	3	0.21	0.1	0.14
(1,2352)	1:B:266:SER:H	1:B:264:PHE:HD2	3	0.21	0.11	0.14
(1,1411)	1:A:234:LEU:H	1:A:233:VAL:HG21	3	0.21	0.06	0.2
(1,1412)	1:B:234:LEU:H	1:B:233:VAL:HG21	3	0.2	0.06	0.2
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE2	3	0.2	0.04	0.22
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE3	3	0.2	0.04	0.22
(1,3342)	1:B:251:ILE:HG21	1:A:264:PHE:HB3	3	0.2	0.04	0.22
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE2	3	0.19	0.05	0.22
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE3	3	0.19	0.05	0.22
(1,3341)	1:A:251:ILE:HG21	1:B:264:PHE:HB3	3	0.19	0.05	0.22
(1,897)	1:A:237:ARG:H	1:A:241:LEU:HD21	3	0.19	0.03	0.2
(1,898)	1:B:237:ARG:H	1:B:241:LEU:HD21	3	0.19	0.03	0.2
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD12	3	0.18	0.06	0.16
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD11	3	0.18	0.06	0.16
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD13	3	0.18	0.06	0.16
(1,304)	1:B:260:ILE:H	1:B:260:ILE:HD11	3	0.18	0.07	0.13
(1,963)	1:A:242:GLN:HE22	1:A:249:VAL:HG11	3	0.18	0.01	0.18
(1,964)	1:B:242:GLN:HE22	1:B:249:VAL:HG11	3	0.18	0.0	0.18
(1,303)	1:A:260:ILE:H	1:A:260:ILE:HD11	3	0.17	0.07	0.13
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB2	3	0.17	0.05	0.14
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB3	3	0.17	0.05	0.14
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB2	3	0.17	0.05	0.13
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB3	3	0.17	0.05	0.13
(1,1211)	1:A:274:LEU:HD11	1:B:237:ARG:HD2	2	0.88	0.0	0.88
(1,1212)	1:B:274:LEU:HD11	1:A:237:ARG:HD2	2	0.88	0.01	0.88
(1,2099)	1:A:257:LYS:H	1:A:257:LYS:HG2	2	0.6	0.42	0.6
(1,2100)	1:B:257:LYS:H	1:B:257:LYS:HG2	2	0.59	0.43	0.59
(1,2963)	1:A:248:THR:HB	1:A:265:PHE:HD2	2	0.42	0.25	0.42
(1,2963)	1:A:248:THR:HB	1:A:245:PHE:HE2	2	0.42	0.25	0.42
(1,2964)	1:B:248:THR:HB	1:B:265:PHE:HD2	2	0.42	0.25	0.42

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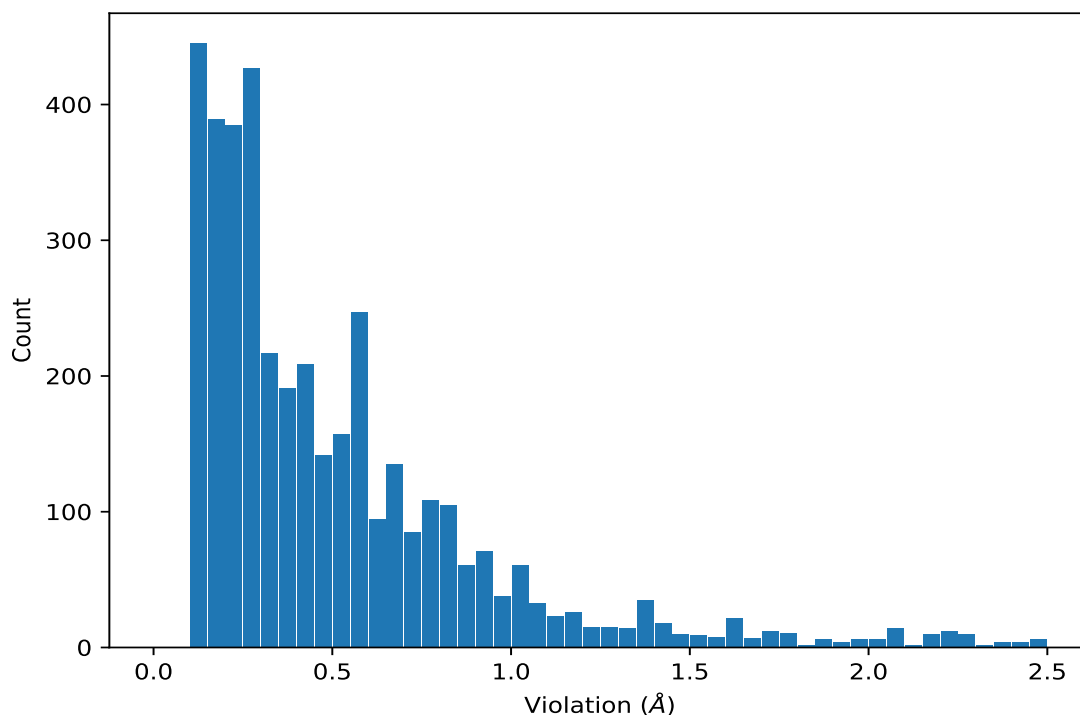
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2964)	1:B:248:THR:HB	1:B:245:PHE:HE2	2	0.42	0.25	0.42
(1,397)	1:A:251:ILE:HG21	1:A:251:ILE:HB	2	0.38	0.28	0.38
(1,3291)	1:A:233:VAL:HG22	1:A:230:LYS:HB3	2	0.31	0.07	0.31
(1,3291)	1:A:233:VAL:HG21	1:A:230:LYS:HB3	2	0.31	0.07	0.31
(1,3291)	1:A:233:VAL:HG23	1:A:230:LYS:HB3	2	0.31	0.07	0.31
(1,3291)	1:A:249:VAL:HG22	1:B:277:LEU:HB3	2	0.31	0.07	0.31
(1,3291)	1:A:249:VAL:HG21	1:B:277:LEU:HB3	2	0.31	0.07	0.31
(1,3291)	1:A:249:VAL:HG23	1:B:277:LEU:HB3	2	0.31	0.07	0.31
(1,3292)	1:B:233:VAL:HG22	1:B:230:LYS:HB3	2	0.31	0.06	0.31
(1,3292)	1:B:233:VAL:HG21	1:B:230:LYS:HB3	2	0.31	0.06	0.31
(1,3292)	1:B:233:VAL:HG23	1:B:230:LYS:HB3	2	0.31	0.06	0.31
(1,3292)	1:B:249:VAL:HG22	1:A:277:LEU:HB3	2	0.31	0.06	0.31
(1,3292)	1:B:249:VAL:HG21	1:A:277:LEU:HB3	2	0.31	0.06	0.31
(1,3292)	1:B:249:VAL:HG23	1:A:277:LEU:HB3	2	0.31	0.06	0.31
(1,1162)	1:B:251:ILE:HD11	1:A:264:PHE:HZ	2	0.3	0.01	0.3
(1,23)	1:A:264:PHE:HE1	1:A:270:LEU:HD11	2	0.29	0.18	0.29
(1,24)	1:B:264:PHE:HE1	1:B:270:LEU:HD11	2	0.29	0.18	0.29
(1,1161)	1:A:251:ILE:HD11	1:B:264:PHE:HZ	2	0.26	0.01	0.26
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD12	2	0.22	0.05	0.22
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD11	2	0.22	0.05	0.22
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD13	2	0.22	0.05	0.22
(1,3068)	1:B:251:ILE:HD11	1:B:234:LEU:HB3	2	0.22	0.12	0.22
(1,3068)	1:B:251:ILE:HD11	1:B:251:ILE:HB	2	0.22	0.12	0.22
(1,2945)	1:A:272:ARG:HE	1:A:269:ASP:HA	2	0.2	0.04	0.2
(1,2946)	1:B:272:ARG:HE	1:B:269:ASP:HA	2	0.2	0.02	0.2
(3,22)	1:A:277:LEU:H	1:A:273:ILE:O	2	0.18	0.04	0.18
(3,46)	1:B:277:LEU:H	1:B:273:ILE:O	2	0.18	0.04	0.18
(1,2662)	1:B:280:ARG:H	1:B:279:GLU:HA	2	0.16	0.01	0.16
(1,2661)	1:A:280:ARG:H	1:A:279:GLU:HA	2	0.15	0.02	0.15
(1,2701)	1:A:282:SER:H	1:A:281:GLU:HB2	2	0.15	0.0	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB2	2	0.15	0.0	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB3	2	0.15	0.0	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG2	2	0.15	0.0	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG3	2	0.15	0.0	0.15
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB2	2	0.15	0.0	0.15
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB3	2	0.15	0.0	0.15
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG2	2	0.15	0.0	0.15
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG3	2	0.15	0.0	0.15
(1,2702)	1:B:282:SER:H	1:B:281:GLU:HB2	2	0.14	0.0	0.14
(1,1399)	1:A:234:LEU:H	1:A:234:LEU:HD21	2	0.12	0.0	0.12
(1,1400)	1:B:234:LEU:H	1:B:234:LEU:HD21	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	1	2.46
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	1	2.46
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	1	2.46
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	1	2.46
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	1	2.46
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	1	2.46
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	2	2.42
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	2	2.42
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	7	2.41
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	7	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	18	2.4
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	18	2.4
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	16	2.35
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	16	2.35
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	2	2.32
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	2	2.31
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	14	2.29
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	3	2.29
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	13	2.29
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	3	2.29
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	13	2.29
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	14	2.28
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	6	2.27
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	6	2.27
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	7	2.25
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	7	2.25
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	4	2.24
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	4	2.24
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	17	2.24
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	17	2.24
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	5	2.22
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	5	2.22
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	8	2.21
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	9	2.21
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	15	2.21
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	8	2.21
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	9	2.21
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	15	2.21
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	18	2.19
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	18	2.18
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	4	2.18
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	2	2.17
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	4	2.17
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	1	2.17
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	14	2.17
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	1	2.17
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	14	2.17
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	2	2.16
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	19	2.12
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	19	2.12
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	11	2.09
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	11	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	6	2.09
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	6	2.09
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	11	2.07
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	11	2.07
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	7	2.07
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	7	2.07
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	3	2.06
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	3	2.06
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	3	2.06
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	3	2.06
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	3	2.06
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	3	2.06
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	20	2.05
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	20	2.05
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	20	2.05
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	20	2.04
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	11	2.04
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	11	2.04
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	10	1.98
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	10	1.98
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	2	1.97
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	2	1.96
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	18	1.96
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	18	1.96
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	18	1.93
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	18	1.93
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	9	1.91
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	9	1.91
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	15	1.87
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	15	1.87
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	12	1.87
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	12	1.87
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	6	1.86
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	6	1.86
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	11	1.82
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	11	1.82
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	7	1.78
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	7	1.78
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	8	1.77
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	8	1.77
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	8	1.77
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	8	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	8	1.77
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	8	1.77
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	2	1.76
(1,1034)	1:B:273:ILE:HG21	1:B:262:ILE:HG12	4	1.76
(1,1033)	1:A:273:ILE:HG21	1:A:262:ILE:HG12	4	1.76
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	14	1.74
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	14	1.74
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	2	1.74
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	15	1.74
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	16	1.73
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	16	1.72
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	8	1.71
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	8	1.71
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	7	1.71
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	7	1.71
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	7	1.71
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	7	1.71
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	15	1.7
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	8	1.67
(2,26)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	1	1.67
(2,25)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	1	1.67
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	7	1.67
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	7	1.66
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	5	1.66
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	5	1.65
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	8	1.64
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	8	1.64
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	8	1.63
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	1	1.63
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	1	1.63
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	8	1.63
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	1	1.62
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	1	1.62
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	1	1.62
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	1	1.62
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	1	1.62
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	1	1.62
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	7	1.62
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	11	1.62
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	19	1.62
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	8	1.62
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	19	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	7	1.61
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	11	1.61
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	12	1.6
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	12	1.6
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	17	1.59
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	17	1.58
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	14	1.57
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	6	1.57
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	14	1.56
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	6	1.56
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	16	1.56
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	16	1.56
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	14	1.53
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	14	1.52
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	4	1.51
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	4	1.51
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	4	1.51
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	4	1.51
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	2	1.5
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	13	1.5
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	2	1.5
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	13	1.49
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	15	1.49
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	15	1.49
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	1	1.47
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	1	1.47
(3,48)	1:B:279:GLU:H	1:B:275:GLU:O	16	1.46
(3,24)	1:A:279:GLU:H	1:A:275:GLU:O	16	1.46
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	11	1.46
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	11	1.46
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	15	1.46
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	11	1.45
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	17	1.45
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	17	1.45
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	11	1.45
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	11	1.45
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	15	1.45
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	11	1.45
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	11	1.44
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	18	1.44
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	11	1.44
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	18	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	1	1.41
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	1	1.41
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	1	1.41
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	5	1.41
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	5	1.41
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	5	1.41
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	5	1.41
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	1	1.4
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	1	1.4
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	1	1.4
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	3	1.4
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	3	1.4
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	3	1.4
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	3	1.4
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	3	1.4
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	3	1.4
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	17	1.4
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	17	1.39
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	18	1.39
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	9	1.39
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	9	1.39
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	18	1.38
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	17	1.38
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	17	1.38
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	17	1.38
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	9	1.38
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	2	1.38
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	2	1.38
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	15	1.37
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	20	1.37
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	9	1.37
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	15	1.36
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	17	1.36
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	17	1.36
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	17	1.36
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	16	1.36
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	16	1.36
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	16	1.36
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	16	1.36
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	20	1.36
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	3	1.35
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	3	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	6	1.34
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	6	1.34
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	16	1.34
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	16	1.34
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	6	1.33
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	5	1.33
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	5	1.33
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	6	1.32
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	17	1.31
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	17	1.31
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	8	1.31
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	8	1.31
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	10	1.3
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	10	1.3
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	12	1.28
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	12	1.27
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	2	1.27
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	2	1.26
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	16	1.26
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	7	1.26
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	10	1.26
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	10	1.26
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	10	1.26
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	10	1.26
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	10	1.26
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	10	1.26
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	16	1.25
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	7	1.25
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	4	1.25
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	3	1.24
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	3	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	12	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	12	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	13	1.24
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	13	1.24
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	12	1.24
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	12	1.24
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	13	1.24
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	13	1.24
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	4	1.22
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	9	1.21
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	17	1.21
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	17	1.21
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	12	1.2
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	14	1.2
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	5	1.2
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	15	1.2
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	15	1.2
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	2	1.2
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	2	1.2
(3,24)	1:A:279:GLU:H	1:A:275:GLU:O	15	1.19
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	12	1.19
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	14	1.19
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	5	1.19
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	1	1.19
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	1	1.19
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	1	1.19
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	1	1.19
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	1	1.19
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	1	1.19
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	14	1.18
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	3	1.18
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	3	1.18
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	3	1.18
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	3	1.18
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	3	1.18
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	3	1.18
(3,48)	1:B:279:GLU:H	1:B:275:GLU:O	15	1.17
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	13	1.16
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	13	1.14
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	20	1.14
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	10	1.14
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	10	1.14
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	14	1.14
(3,48)	1:B:279:GLU:H	1:B:275:GLU:O	9	1.13
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	2	1.13
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	2	1.13
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	20	1.13
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	10	1.13
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	10	1.13
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	9	1.13
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	9	1.13
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	3	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,24)	1:A:279:GLU:H	1:A:275:GLU:O	9	1.12
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	3	1.12
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	16	1.1
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	6	1.1
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	9	1.1
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	9	1.1
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	10	1.1
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	10	1.1
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	6	1.1
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	10	1.09
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	17	1.09
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	15	1.09
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	15	1.09
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	15	1.09
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	15	1.09
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	11	1.09
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	11	1.09
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	10	1.08
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	16	1.08
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	17	1.08
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	19	1.08
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	19	1.08
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	8	1.08
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	8	1.08
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	8	1.08
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	8	1.08
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	8	1.08
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	8	1.08
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	17	1.08
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	17	1.08
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	17	1.08
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	4	1.07
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	4	1.07
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	11	1.07
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	19	1.06
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	19	1.06
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	1	1.05
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	10	1.05
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	10	1.05
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	4	1.05
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	4	1.05
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	7	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	18	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	18	1.04
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	18	1.04
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	18	1.04
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	18	1.04
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	18	1.04
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	1	1.04
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	17	1.04
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	17	1.04
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	17	1.04
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	1	1.04
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	1	1.04
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	20	1.04
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	20	1.04
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	7	1.04
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	9	1.03
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	4	1.03
(1,376)	1:B:262:ILE:HG21	1:B:245:PHE:HB2	11	1.03
(1,375)	1:A:262:ILE:HG21	1:A:245:PHE:HB2	11	1.03
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	11	1.03
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	9	1.02
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	4	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	1	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	1	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	1	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	4	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	4	1.02
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	4	1.02
(1,2100)	1:B:257:LYS:H	1:B:257:LYS:HG2	13	1.02
(1,2099)	1:A:257:LYS:H	1:A:257:LYS:HG2	13	1.02
(1,974)	1:B:247:THR:HG21	1:B:273:ILE:HD12	18	1.01
(1,974)	1:B:247:THR:HG21	1:B:273:ILE:HD11	18	1.01
(1,974)	1:B:247:THR:HG21	1:B:273:ILE:HD13	18	1.01
(1,973)	1:A:247:THR:HG21	1:A:273:ILE:HD12	18	1.01
(1,973)	1:A:247:THR:HG21	1:A:273:ILE:HD11	18	1.01
(1,973)	1:A:247:THR:HG21	1:A:273:ILE:HD13	18	1.01
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	20	1.01
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	1	1.01
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	1	1.01
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	1	1.01
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	8	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	8	1.01
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	8	1.01
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	8	1.01
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	8	1.01
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	8	1.01
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	8	1.0
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	11	1.0
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	11	1.0
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	11	1.0
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	11	1.0
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	11	1.0
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	11	1.0
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	18	1.0
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	18	1.0
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	18	1.0
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	18	1.0
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	20	1.0
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	3	1.0
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	3	1.0
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	8	0.99
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	16	0.99
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	16	0.99
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	13	0.99
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	13	0.99
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	16	0.99
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	1	0.99
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	1	0.99
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	9	0.98
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	9	0.98
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	9	0.98
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	9	0.98
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	9	0.98
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	9	0.98
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	18	0.97
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	18	0.97
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	8	0.97
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	9	0.97
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	16	0.97
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	9	0.97
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	16	0.97
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	11	0.96
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	11	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	4	0.96
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	5	0.96
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	5	0.96
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	5	0.96
(1,352)	1:B:273:ILE:HD11	1:B:264:PHE:HB3	4	0.96
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	18	0.96
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	18	0.96
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	8	0.96
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	1	0.96
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	1	0.96
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	16	0.96
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	14	0.96
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	14	0.96
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	9	0.96
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	9	0.96
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	4	0.95
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	19	0.95
(1,351)	1:A:273:ILE:HD11	1:A:264:PHE:HB3	4	0.95
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	15	0.95
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	15	0.95
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	13	0.94
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	19	0.94
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	5	0.94
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	5	0.94
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	5	0.94
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	3	0.94
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	3	0.94
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	9	0.94
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	9	0.94
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	9	0.94
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	9	0.94
(1,2693)	1:A:282:SER:H	1:A:280:ARG:HD3	2	0.94
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	7	0.94
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	7	0.94
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	20	0.94
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	6	0.94
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	20	0.94
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	13	0.94
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	20	0.93
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	20	0.93
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	1	0.93
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	17	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	1	0.93
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	17	0.93
(1,2694)	1:B:282:SER:H	1:B:280:ARG:HD3	2	0.93
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	7	0.93
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	7	0.93
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	4	0.93
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD12	1	0.93
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD11	1	0.93
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD13	1	0.93
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	1	0.92
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	17	0.92
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	17	0.92
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	2	0.92
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	6	0.92
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	5	0.92
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	6	0.92
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	4	0.92
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD12	1	0.92
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD11	1	0.92
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD13	1	0.92
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	6	0.92
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	6	0.92
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	6	0.92
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	6	0.92
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	6	0.92
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	6	0.92
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	2	0.91
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	5	0.91
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	5	0.91
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	16	0.91
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	6	0.91
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	9	0.9
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	9	0.9
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	1	0.9
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	7	0.9
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	7	0.9
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	7	0.9
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	8	0.9
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	8	0.9
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	16	0.9
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	5	0.9
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	5	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	5	0.9
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	13	0.9
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	7	0.89
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	7	0.89
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	7	0.89
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	12	0.89
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	12	0.89
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	12	0.89
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	6	0.89
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	6	0.89
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	6	0.89
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	6	0.89
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	13	0.89
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	9	0.88
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	9	0.88
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	12	0.88
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	12	0.88
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	12	0.88
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	10	0.88
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	16	0.88
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	20	0.88
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	8	0.88
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	10	0.88
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	16	0.88
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	20	0.88
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	8	0.88
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	8	0.88
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	17	0.88
(1,1212)	1:B:274:LEU:HD11	1:A:237:ARG:HD2	8	0.88
(1,1211)	1:A:274:LEU:HD11	1:B:237:ARG:HD2	8	0.88
(1,1211)	1:A:274:LEU:HD11	1:B:237:ARG:HD2	11	0.88
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	10	0.88
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	3	0.87
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	3	0.87
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	20	0.87
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	20	0.87
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	8	0.87
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	12	0.87
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	14	0.87
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	14	0.87
(1,376)	1:B:262:ILE:HG21	1:B:245:PHE:HB2	3	0.87
(1,375)	1:A:262:ILE:HG21	1:A:245:PHE:HB2	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	11	0.87
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	15	0.87
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	17	0.87
(1,1349)	1:A:230:LYS:H	1:A:230:LYS:HB2	6	0.87
(1,1212)	1:B:274:LEU:HD11	1:A:237:ARG:HD2	11	0.87
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	10	0.86
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	3	0.86
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	3	0.86
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	3	0.86
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	6	0.86
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	15	0.86
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	6	0.86
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	12	0.86
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	15	0.86
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	11	0.86
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	11	0.86
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	11	0.86
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	4	0.86
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	4	0.86
(1,1350)	1:B:230:LYS:H	1:B:230:LYS:HB2	6	0.86
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	10	0.86
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	4	0.85
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	2	0.85
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	5	0.85
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	7	0.85
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	19	0.85
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	2	0.85
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	5	0.85
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	7	0.85
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	19	0.85
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	19	0.85
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	19	0.85
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	12	0.85
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	12	0.85
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	12	0.85
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	12	0.85
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	3	0.85
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	3	0.85
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	3	0.84
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	3	0.84
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	3	0.84
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	9	0.84
(1,378)	1:B:262:ILE:HG21	1:B:262:ILE:HG12	13	0.84
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	4	0.84
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	9	0.84
(1,377)	1:A:262:ILE:HG21	1:A:262:ILE:HG12	13	0.84
(1,376)	1:B:262:ILE:HG21	1:B:245:PHE:HB2	17	0.84
(1,375)	1:A:262:ILE:HG21	1:A:245:PHE:HB2	17	0.84
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	17	0.84
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	17	0.84
(1,2934)	1:B:237:ARG:HE	1:B:233:VAL:HG12	11	0.84
(1,2934)	1:B:237:ARG:HE	1:B:233:VAL:HG11	11	0.84
(1,2934)	1:B:237:ARG:HE	1:B:233:VAL:HG13	11	0.84
(1,2933)	1:A:237:ARG:HE	1:A:233:VAL:HG12	11	0.84
(1,2933)	1:A:237:ARG:HE	1:A:233:VAL:HG11	11	0.84
(1,2933)	1:A:237:ARG:HE	1:A:233:VAL:HG13	11	0.84
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	15	0.84
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	16	0.84
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	16	0.84
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	16	0.83
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	10	0.83
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	10	0.83
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	10	0.83
(1,3302)	1:B:232:ALA:HB1	1:B:230:LYS:HB3	1	0.83
(1,3302)	1:B:232:ALA:HB1	1:B:235:LYS:HB2	1	0.83
(1,3301)	1:A:232:ALA:HB1	1:A:230:LYS:HB3	1	0.83
(1,3301)	1:A:232:ALA:HB1	1:A:235:LYS:HB2	1	0.83
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	15	0.83
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	15	0.83
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	16	0.83
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	16	0.83
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	17	0.83
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	17	0.83
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	17	0.83
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	17	0.83
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	17	0.83
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	17	0.83
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	3	0.82
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	11	0.82
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	11	0.82
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	11	0.82
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	11	0.82
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	16	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	4	0.82
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	8	0.82
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	4	0.82
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	4	0.82
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	13	0.81
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	13	0.81
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	10	0.81
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	10	0.81
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	8	0.81
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	20	0.81
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	20	0.81
(1,1350)	1:B:230:LYS:H	1:B:230:LYS:HB2	1	0.81
(1,1349)	1:A:230:LYS:H	1:A:230:LYS:HB2	1	0.81
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	16	0.81
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	16	0.81
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	16	0.81
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	19	0.81
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	19	0.81
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	19	0.81
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	14	0.8
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	14	0.8
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	14	0.8
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	14	0.8
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	14	0.8
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	7	0.8
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	7	0.8
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	8	0.8
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	8	0.8
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	11	0.8
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	11	0.8
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	11	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	11	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	11	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	11	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	16	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	16	0.8
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	16	0.8
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	11	0.8
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	11	0.8
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	19	0.8
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	19	0.8
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	17	0.79
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	17	0.79
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	17	0.79
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	17	0.79
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	5	0.79
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	5	0.79
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	1	0.79
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	8	0.79
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	18	0.79
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	19	0.79
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	1	0.79
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	8	0.79
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	18	0.79
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	19	0.79
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	6	0.79
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	6	0.79
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	20	0.79
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	20	0.79
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	20	0.79
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	3	0.78
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	17	0.78
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	17	0.78
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	14	0.78
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	14	0.78
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	14	0.78
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	17	0.78
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	17	0.78
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	8	0.78
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	8	0.78
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	6	0.78
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	20	0.78
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	20	0.78
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	20	0.78
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	7	0.77
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	6	0.77
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	11	0.77
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	12	0.77
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	6	0.77
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	11	0.77
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	12	0.77
(1,2658)	1:B:279:GLU:H	1:B:278:SER:HB2	8	0.77
(1,2657)	1:A:279:GLU:H	1:A:278:SER:HB2	8	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:B:230:LYS:H	1:B:230:LYS:HB2	19	0.77
(1,1349)	1:A:230:LYS:H	1:A:230:LYS:HB2	19	0.77
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	6	0.77
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	7	0.77
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	19	0.76
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	8	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	15	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	15	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	15	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	18	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	18	0.76
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	18	0.76
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	7	0.76
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	14	0.76
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	9	0.76
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	9	0.76
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	9	0.76
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	3	0.76
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	10	0.76
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	3	0.76
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	8	0.76
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	8	0.76
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	19	0.76
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	19	0.76
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	19	0.76
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	19	0.76
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	19	0.76
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	19	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	4	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	4	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	4	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	5	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	5	0.76
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	5	0.76
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	17	0.75
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	3	0.75
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	3	0.75
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	19	0.75
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	17	0.75
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	17	0.75
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	17	0.75
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	20	0.75
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	20	0.75
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	20	0.75
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	20	0.75
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	20	0.75
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	20	0.75
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	19	0.75
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	19	0.75
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	14	0.75
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	8	0.75
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	9	0.75
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	9	0.75
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	9	0.75
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	20	0.75
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	10	0.75
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	20	0.75
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	16	0.75
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	20	0.75
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	16	0.75
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	5	0.75
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	5	0.75
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	5	0.75
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	16	0.75
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	16	0.75
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	16	0.75
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	5	0.74
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	5	0.74
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	13	0.74
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	13	0.74
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	13	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	13	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	13	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	13	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	18	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	18	0.74
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	18	0.74
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	8	0.74
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	4	0.74
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	14	0.74
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	13	0.74
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	20	0.74
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	17	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	17	0.74
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	17	0.74
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	17	0.74
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	17	0.74
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	17	0.74
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	7	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	4	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	4	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	4	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	16	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	16	0.74
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	16	0.74
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	12	0.73
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	3	0.73
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	3	0.73
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	19	0.73
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	19	0.73
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	19	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	6	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	6	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	6	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	15	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	15	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	15	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	19	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	19	0.73
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	19	0.73
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	5	0.73
(1,2674)	1:B:280:ARG:H	1:B:280:ARG:HB2	13	0.73
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	4	0.73
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	5	0.73
(1,2673)	1:A:280:ARG:H	1:A:280:ARG:HB2	14	0.73
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	14	0.73
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	14	0.73
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	10	0.73
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	10	0.73
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	10	0.73
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	10	0.73
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	10	0.73
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	10	0.73
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	12	0.72
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	10	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	17	0.72
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	17	0.72
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	2	0.72
(1,1190)	1:B:276:LEU:HD11	1:B:245:PHE:HE1	17	0.72
(1,1189)	1:A:276:LEU:HD11	1:A:245:PHE:HE1	17	0.72
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	12	0.71
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	12	0.71
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	8	0.71
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	6	0.71
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	6	0.71
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	6	0.71
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	17	0.71
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	17	0.71
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	2	0.71
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	6	0.71
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	1	0.71
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	1	0.71
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	1	0.71
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	16	0.71
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	16	0.71
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	12	0.71
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	12	0.71
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	12	0.71
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	12	0.71
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	12	0.71
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	12	0.71
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	8	0.7
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	8	0.7
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	8	0.7
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	6	0.7
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	20	0.7
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	20	0.7
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	1	0.7
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	1	0.7
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	1	0.7
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	10	0.7
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	10	0.7
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	13	0.7
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	13	0.7
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	13	0.7
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	12	0.7
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	12	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	1	0.7
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	1	0.7
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	1	0.7
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	1	0.7
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	1	0.7
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	1	0.7
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	10	0.69
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	8	0.69
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	8	0.69
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	8	0.69
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD12	3	0.69
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD11	3	0.69
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD13	3	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD12	3	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD11	3	0.69
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD13	3	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	7	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	7	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	7	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	10	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	10	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	10	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	18	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	18	0.69
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	18	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	7	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	7	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	7	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	10	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	10	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	10	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	13	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	13	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	13	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	18	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	18	0.69
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	18	0.69
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	9	0.68
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	10	0.68
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	11	0.68
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	11	0.68
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	15	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	15	0.68
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	8	0.68
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	8	0.68
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	8	0.68
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	6	0.68
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	9	0.68
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	9	0.68
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	2	0.68
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	2	0.68
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	2	0.68
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	2	0.68
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	2	0.68
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	2	0.68
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	6	0.67
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	6	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	2	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	2	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	2	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	11	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	11	0.67
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	11	0.67
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	2	0.67
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	2	0.67
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	2	0.67
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	5	0.67
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	5	0.67
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	5	0.67
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	5	0.67
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	1	0.67
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	1	0.67
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	1	0.67
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	1	0.67
(1,2964)	1:B:248:THR:HB	1:B:265:PHE:HD2	12	0.67
(1,2964)	1:B:248:THR:HB	1:B:245:PHE:HE2	12	0.67
(1,2963)	1:A:248:THR:HB	1:A:265:PHE:HD2	12	0.67
(1,2963)	1:A:248:THR:HB	1:A:245:PHE:HE2	12	0.67
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	9	0.67
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	8	0.67
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	8	0.67
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	8	0.67
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	15	0.67
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	15	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	15	0.67
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	15	0.67
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	15	0.67
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	15	0.67
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	10	0.66
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	15	0.66
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	13	0.66
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	9	0.66
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	17	0.66
(1,398)	1:B:251:ILE:HG21	1:B:251:ILE:HB	10	0.66
(1,397)	1:A:251:ILE:HG21	1:A:251:ILE:HB	10	0.66
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	16	0.66
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	16	0.66
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	13	0.66
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	13	0.66
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	5	0.66
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	5	0.66
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	9	0.66
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	8	0.66
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	8	0.66
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	8	0.66
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	14	0.66
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	14	0.66
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	15	0.65
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	6	0.65
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	6	0.65
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	3	0.65
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	11	0.65
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	11	0.65
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	11	0.65
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	12	0.65
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	12	0.65
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	15	0.65
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	15	0.65
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	6	0.65
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	1	0.64
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	16	0.64
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	13	0.64
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	6	0.64
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	6	0.64
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	16	0.64
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	16	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	8	0.64
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	10	0.64
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	17	0.64
(1,422)	1:B:259:LYS:HE2	1:B:261:GLU:HG3	3	0.64
(1,422)	1:B:259:LYS:HE3	1:B:261:GLU:HG3	3	0.64
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	9	0.64
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	9	0.64
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	9	0.64
(1,364)	1:B:262:ILE:HG21	1:B:245:PHE:HB3	11	0.64
(1,363)	1:A:262:ILE:HG21	1:A:245:PHE:HB3	11	0.64
(1,3301)	1:A:232:ALA:HB1	1:A:230:LYS:HB3	6	0.64
(1,3301)	1:A:232:ALA:HB1	1:A:235:LYS:HB2	6	0.64
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	5	0.64
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	5	0.64
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	7	0.64
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	1	0.63
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	16	0.63
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	16	0.63
(2,26)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	3	0.63
(2,25)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	3	0.63
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	8	0.63
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	3	0.63
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	16	0.63
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	16	0.63
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	9	0.63
(1,3302)	1:B:232:ALA:HB1	1:B:230:LYS:HB3	6	0.63
(1,3302)	1:B:232:ALA:HB1	1:B:235:LYS:HB2	6	0.63
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	5	0.63
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	5	0.63
(1,286)	1:B:270:LEU:HA	1:B:270:LEU:HD11	10	0.63
(1,285)	1:A:270:LEU:HA	1:A:270:LEU:HD11	10	0.63
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	8	0.63
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	4	0.63
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	4	0.63
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	4	0.63
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	4	0.63
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	14	0.63
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	3	0.63
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	3	0.63
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	7	0.63
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	7	0.62
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	7	0.62
(1,840)	1:B:270:LEU:HD21	1:B:270:LEU:HB3	4	0.62
(1,839)	1:A:270:LEU:HD21	1:A:270:LEU:HB3	4	0.62
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	7	0.62
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	10	0.62
(1,421)	1:A:259:LYS:HE2	1:A:261:GLU:HG3	3	0.62
(1,421)	1:A:259:LYS:HE3	1:A:261:GLU:HG3	3	0.62
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	8	0.62
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	8	0.62
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	8	0.62
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	8	0.62
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	7	0.62
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	7	0.62
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	3	0.62
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	3	0.62
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	12	0.62
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	8	0.62
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	15	0.62
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	15	0.62
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	14	0.62
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	15	0.62
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	2	0.61
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	3	0.61
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	16	0.61
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	2	0.61
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	10	0.61
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	10	0.61
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	16	0.61
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	16	0.61
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	16	0.61
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	2	0.61
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	7	0.61
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	7	0.61
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	16	0.61
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	16	0.61
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	16	0.61
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	12	0.61
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	17	0.61
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	17	0.61
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	12	0.61
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	15	0.61
(1,1196)	1:B:276:LEU:HD21	1:B:245:PHE:HE1	17	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:A:276:LEU:HD21	1:A:245:PHE:HE1	17	0.61
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	3	0.61
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	3	0.61
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	3	0.61
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	13	0.6
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	13	0.6
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	13	0.6
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	6	0.6
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	15	0.6
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	15	0.6
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	7	0.6
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	16	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	3	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	3	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	11	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	11	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	18	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	18	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	19	0.6
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	19	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	3	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	3	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	11	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	11	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	18	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	18	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	19	0.6
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	19	0.6
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	7	0.6
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	16	0.6
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	16	0.6
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	16	0.6
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	2	0.6
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	4	0.6
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	4	0.6
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG2	12	0.6
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG3	12	0.6
(1,3129)	1:A:236:GLU:HG2	1:A:234:LEU:HB2	12	0.6
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	16	0.6
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	16	0.6
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	16	0.6
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD22	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD21	7	0.6
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD23	7	0.6
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	12	0.6
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	12	0.6
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	18	0.6
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	12	0.6
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	18	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	9	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	9	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	9	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	14	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	14	0.6
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	14	0.6
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	14	0.6
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	14	0.6
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	14	0.6
(1,1190)	1:B:276:LEU:HD11	1:B:245:PHE:HE1	11	0.6
(1,1189)	1:A:276:LEU:HD11	1:A:245:PHE:HE1	11	0.6
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	3	0.6
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	3	0.6
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	3	0.6
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	7	0.59
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	7	0.59
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	6	0.59
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	16	0.59
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	19	0.59
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	16	0.59
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	16	0.59
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	16	0.59
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	16	0.59
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	16	0.59
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	16	0.59
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	16	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	2	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	2	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	5	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	5	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	14	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	14	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG2	16	0.59
(1,426)	1:B:259:LYS:HE3	1:B:259:LYS:HG3	16	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	2	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	5	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	5	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	14	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	14	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG2	16	0.59
(1,425)	1:A:259:LYS:HE3	1:A:259:LYS:HG3	16	0.59
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	14	0.59
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	7	0.59
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	14	0.59
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	17	0.59
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	17	0.59
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG2	12	0.59
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG3	12	0.59
(1,3130)	1:B:236:GLU:HG2	1:B:234:LEU:HB2	12	0.59
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG2	15	0.59
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG3	15	0.59
(1,3129)	1:A:236:GLU:HG2	1:A:234:LEU:HB2	15	0.59
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	20	0.59
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	20	0.59
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	20	0.59
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	20	0.59
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	20	0.59
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	20	0.59
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	9	0.59
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	3	0.59
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	12	0.59
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	12	0.59
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	12	0.59
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	9	0.59
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	9	0.59
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	10	0.59
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	9	0.59
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	9	0.59
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	9	0.59
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	4	0.59
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	14	0.58
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	16	0.58
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	4	0.58
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	4	0.58
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	4	0.58
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG2	15	0.58
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG3	15	0.58
(1,3130)	1:B:236:GLU:HG2	1:B:234:LEU:HB2	15	0.58
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	10	0.58
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	10	0.58
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	10	0.58
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	10	0.58
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	16	0.58
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	20	0.58
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	20	0.58
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	20	0.58
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	20	0.58
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	20	0.58
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	20	0.58
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD12	1	0.58
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD11	1	0.58
(1,2778)	1:B:244:TYR:H	1:B:276:LEU:HD13	1	0.58
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD12	1	0.58
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD11	1	0.58
(1,2777)	1:A:244:TYR:H	1:A:276:LEU:HD13	1	0.58
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	2	0.58
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	3	0.58
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	9	0.58
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	15	0.58
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	15	0.58
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	10	0.58
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	4	0.58
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	17	0.58
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	16	0.58
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	10	0.57
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	1	0.57
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	13	0.57
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	13	0.57
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	13	0.57
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	13	0.57
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	13	0.57
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	13	0.57
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	13	0.57
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	5	0.57
(1,328)	1:B:251:ILE:HD11	1:B:238:GLU:HG3	1	0.57
(1,327)	1:A:251:ILE:HD11	1:A:238:GLU:HG3	1	0.57
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	16	0.57
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD22	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD21	7	0.57
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD23	7	0.57
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	2	0.57
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	12	0.57
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	12	0.57
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	12	0.57
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	18	0.57
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	19	0.57
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	19	0.57
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	15	0.56
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	11	0.56
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	11	0.56
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	14	0.56
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	19	0.56
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	1	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	14	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	14	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	14	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	15	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	15	0.56
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	15	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	14	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	14	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	14	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	15	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	15	0.56
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	15	0.56
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	3	0.56
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	5	0.56
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	5	0.56
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG2	11	0.56
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG3	11	0.56
(1,3129)	1:A:236:GLU:HG2	1:A:234:LEU:HB2	11	0.56
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD22	3	0.56
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD21	3	0.56
(1,257)	1:A:237:ARG:HD2	1:B:270:LEU:HD23	3	0.56
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	4	0.56
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	12	0.56
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	20	0.56
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	20	0.56
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	18	0.56
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	16	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	7	0.56
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	7	0.56
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	7	0.56
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	7	0.56
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	7	0.56
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	7	0.56
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	10	0.55
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	4	0.55
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	13	0.55
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	13	0.55
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	17	0.55
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	17	0.55
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	1	0.55
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	1	0.55
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	17	0.55
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	17	0.55
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	17	0.55
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	17	0.55
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	17	0.55
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	17	0.55
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	3	0.55
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	2	0.55
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	2	0.55
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	2	0.55
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	2	0.55
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	12	0.55
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	12	0.55
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	8	0.55
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	5	0.55
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	5	0.55
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG2	11	0.55
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG3	11	0.55
(1,3130)	1:B:236:GLU:HG2	1:B:234:LEU:HB2	11	0.55
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	19	0.55
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	20	0.55
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	20	0.55
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	20	0.55
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	20	0.55
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	20	0.55
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	20	0.55
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	17	0.55
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	4	0.54
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	4	0.54
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	13	0.54
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	15	0.54
(2,26)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	10	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	2	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	5	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	6	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	7	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	9	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	11	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	12	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	13	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	14	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	15	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	16	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	18	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	19	0.54
(1,836)	1:B:270:LEU:HD21	1:B:270:LEU:HG	20	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	2	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	5	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	6	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	7	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	9	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	11	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	12	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	13	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	14	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	15	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	16	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	18	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	19	0.54
(1,835)	1:A:270:LEU:HD21	1:A:270:LEU:HG	20	0.54
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	5	0.54
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	18	0.54
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	18	0.54
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	20	0.54
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	20	0.54
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	8	0.54
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	15	0.54
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	15	0.54
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	15	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	15	0.54
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD22	3	0.54
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD21	3	0.54
(1,258)	1:B:237:ARG:HD2	1:A:270:LEU:HD23	3	0.54
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	4	0.54
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	12	0.54
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	19	0.54
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	4	0.53
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	17	0.53
(2,25)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	10	0.53
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	2	0.53
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	13	0.53
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	13	0.53
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	1	0.53
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	1	0.53
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	13	0.53
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	13	0.53
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	18	0.53
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	18	0.53
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	19	0.53
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	19	0.53
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	20	0.53
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	20	0.53
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	1	0.53
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	1	0.53
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	13	0.53
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	13	0.53
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	19	0.53
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	19	0.53
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	8	0.53
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	8	0.53
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	6	0.53
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	6	0.53
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	17	0.53
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	17	0.53
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG2	9	0.53
(1,3129)	1:A:236:GLU:HG2	1:A:253:ARG:HG3	9	0.53
(1,3129)	1:A:236:GLU:HG2	1:A:234:LEU:HB2	9	0.53
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HD1	18	0.53
(1,3072)	1:B:262:ILE:HG21	1:B:264:PHE:HE1	18	0.53
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HD1	18	0.53
(1,3071)	1:A:262:ILE:HG21	1:A:264:PHE:HE1	18	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	1	0.53
(1,1190)	1:B:276:LEU:HD11	1:B:245:PHE:HE1	3	0.53
(1,1189)	1:A:276:LEU:HD11	1:A:245:PHE:HE1	3	0.53
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	13	0.52
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	17	0.52
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	6	0.52
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	13	0.52
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	2	0.52
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	20	0.52
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	4	0.52
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	4	0.52
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	6	0.52
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	6	0.52
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	17	0.52
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	17	0.52
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	8	0.52
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	8	0.52
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG2	9	0.52
(1,3130)	1:B:236:GLU:HG2	1:B:253:ARG:HG3	9	0.52
(1,3130)	1:B:236:GLU:HG2	1:B:234:LEU:HB2	9	0.52
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	1	0.52
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	10	0.51
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	1	0.51
(1,340)	1:B:273:ILE:HD11	1:B:270:LEU:HA	4	0.51
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	8	0.51
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	8	0.51
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	1	0.51
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	1	0.51
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	4	0.51
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	4	0.51
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	10	0.51
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	10	0.51
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	2	0.51
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	5	0.51
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	7	0.51
(1,1119)	1:A:279:GLU:HB2	1:B:276:LEU:HD22	16	0.51
(1,1119)	1:A:279:GLU:HB2	1:B:276:LEU:HD21	16	0.51
(1,1119)	1:A:279:GLU:HB2	1:B:276:LEU:HD23	16	0.51
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	10	0.5
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	18	0.5
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	18	0.5
(1,692)	1:B:229:VAL:HB	1:B:229:VAL:H	18	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	18	0.5
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	18	0.5
(1,691)	1:A:229:VAL:HB	1:A:229:VAL:H	18	0.5
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	1	0.5
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	17	0.5
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	7	0.5
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	7	0.5
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	7	0.5
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	7	0.5
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	12	0.5
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	12	0.5
(1,339)	1:A:273:ILE:HD11	1:A:270:LEU:HA	4	0.5
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	2	0.5
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	2	0.5
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	20	0.5
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	20	0.5
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	20	0.5
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	20	0.5
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	10	0.5
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	14	0.5
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	14	0.5
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	2	0.5
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	5	0.5
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	6	0.5
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	6	0.5
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	7	0.5
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	6	0.5
(1,1120)	1:B:279:GLU:HB2	1:A:276:LEU:HD22	16	0.5
(1,1120)	1:B:279:GLU:HB2	1:A:276:LEU:HD21	16	0.5
(1,1120)	1:B:279:GLU:HB2	1:A:276:LEU:HD23	16	0.5
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	20	0.49
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	3	0.49
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	3	0.49
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	12	0.49
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	12	0.49
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	3	0.49
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	3	0.49
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	2	0.49
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	2	0.49
(1,2682)	1:B:281:GLU:H	1:B:280:ARG:HD3	5	0.49
(1,2681)	1:A:281:GLU:H	1:A:280:ARG:HD3	5	0.49
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	2	0.49
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	10	0.49
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	12	0.49
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	15	0.49
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	12	0.49
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	15	0.49
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	20	0.49
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	20	0.49
(3,32)	1:B:249:VAL:H	1:B:242:GLN:OE1	18	0.48
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	11	0.48
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	11	0.48
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	8	0.48
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	8	0.48
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	17	0.48
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	8	0.48
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	17	0.48
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	5	0.48
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	5	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	2	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	5	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	7	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	12	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	16	0.48
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	19	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	2	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	5	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	7	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	12	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	16	0.48
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	19	0.48
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	10	0.48
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	10	0.48
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	6	0.48
(3,8)	1:A:249:VAL:H	1:A:242:GLN:OE1	18	0.47
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	12	0.47
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	18	0.47
(2,28)	1:B:241:LEU:HD21	1:B:245:PHE:HE2	7	0.47
(2,27)	1:A:241:LEU:HD21	1:A:245:PHE:HE2	7	0.47
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	11	0.47
(1,886)	1:B:261:GLU:HG3	1:B:252:LYS:HG3	18	0.47
(1,885)	1:A:261:GLU:HG3	1:A:252:LYS:HG3	18	0.47
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	7	0.47
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	7	0.47
(1,30)	1:B:240:TYR:HE1	1:B:244:TYR:HB3	1	0.47
(1,29)	1:A:240:TYR:HE1	1:A:244:TYR:HB3	1	0.47
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	11	0.47
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	8	0.47
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	9	0.47
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	9	0.47
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	2	0.47
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	2	0.47
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	19	0.47
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	4	0.46
(1,998)	1:B:247:THR:HG21	1:B:245:PHE:HB3	13	0.46
(1,997)	1:A:247:THR:HG21	1:A:245:PHE:HB3	13	0.46
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	5	0.46
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	2	0.46
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	6	0.46
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	18	0.46
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	2	0.46
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	6	0.46
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	18	0.46
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	18	0.46
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	18	0.46
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	17	0.46
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	10	0.46
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	10	0.46
(1,370)	1:B:263:GLU:H	1:B:262:ILE:HG21	15	0.46
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	3	0.46
(1,24)	1:B:264:PHE:HE1	1:B:270:LEU:HD11	4	0.46
(1,23)	1:A:264:PHE:HE1	1:A:270:LEU:HD11	4	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	1	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	3	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	4	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	8	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	9	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	13	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	14	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	15	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	17	0.46
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	18	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	1	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	4	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	8	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	9	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	11	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	14	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	15	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	17	0.46
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	18	0.46
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	13	0.46
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	13	0.46
(1,1192)	1:B:276:LEU:HD11	1:B:245:PHE:HD1	16	0.46
(1,1191)	1:A:276:LEU:HD11	1:A:245:PHE:HD1	16	0.46
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	2	0.46
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	12	0.45
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	5	0.45
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	4	0.45
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	4	0.45
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	5	0.45
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	18	0.45
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	15	0.45
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	15	0.45
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	15	0.45
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	8	0.45
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	8	0.45
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	9	0.45
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	9	0.45
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	9	0.45
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	9	0.45
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	10	0.45
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	10	0.45
(1,369)	1:A:263:GLU:H	1:A:262:ILE:HG21	15	0.45
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	3	0.45
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	10	0.45
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	10	0.45
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	14	0.45
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	14	0.45
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	14	0.45
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	1	0.45
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	10	0.45
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	1	0.45
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	10	0.45
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	13	0.45
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	6	0.45
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	20	0.45
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	18	0.45
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	4	0.44
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	1	0.44
(1,982)	1:B:263:GLU:H	1:B:247:THR:HG21	18	0.44
(1,981)	1:A:263:GLU:H	1:A:247:THR:HG21	18	0.44
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	9	0.44
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	9	0.44
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	9	0.44
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	9	0.44
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	9	0.44
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	9	0.44
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	9	0.44
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	9	0.44
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	9	0.44
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG22	1	0.44
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG21	1	0.44
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG23	1	0.44
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD12	1	0.44
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD11	1	0.44
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD13	1	0.44
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG22	1	0.44
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG21	1	0.44
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG23	1	0.44
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD12	1	0.44
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD11	1	0.44
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD13	1	0.44
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	16	0.44
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	16	0.44
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	16	0.44
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	14	0.44
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	14	0.44
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	14	0.44
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	6	0.44
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	6	0.44
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	10	0.44
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	11	0.44
(1,1662)	1:B:243:ASN:H	1:B:243:ASN:HB3	20	0.44
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	10	0.44
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:A:243:ASN:H	1:A:243:ASN:HB3	20	0.44
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	9	0.44
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	9	0.44
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	2	0.44
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	13	0.44
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	13	0.44
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	13	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	13	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	13	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	13	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	18	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	18	0.44
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	18	0.44
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	13	0.43
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	1	0.43
(1,920)	1:B:276:LEU:HD11	1:B:244:TYR:HD2	8	0.43
(1,919)	1:A:276:LEU:HD11	1:A:244:TYR:HD2	8	0.43
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	12	0.43
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	12	0.43
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	12	0.43
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	9	0.43
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	10	0.43
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	10	0.43
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	13	0.43
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	1	0.43
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	1	0.43
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	16	0.43
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	16	0.43
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	16	0.43
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	13	0.43
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	13	0.43
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	13	0.43
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	11	0.43
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	19	0.43
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	7	0.43
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	11	0.43
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	18	0.43
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	19	0.43
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	6	0.43
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	13	0.43
(1,1213)	1:A:274:LEU:HD11	1:B:237:ARG:HD3	8	0.43
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	13	0.42
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	4	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	12	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	12	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	12	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	15	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	15	0.42
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	15	0.42
(1,758)	1:B:260:ILE:HG13	1:A:264:PHE:HE2	6	0.42
(1,757)	1:A:260:ILE:HG13	1:B:264:PHE:HE2	6	0.42
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	13	0.42
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	17	0.42
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	20	0.42
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	20	0.42
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	14	0.42
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	14	0.42
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	14	0.42
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	14	0.42
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	1	0.42
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	1	0.42
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	6	0.42
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	6	0.42
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	6	0.42
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	6	0.42
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	16	0.42
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	16	0.42
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	16	0.42
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	1	0.42
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	13	0.42
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	13	0.42
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	13	0.42
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	7	0.42
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	14	0.42
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	18	0.42
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	20	0.42
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	14	0.42
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	20	0.42
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	3	0.42
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG21	10	0.42
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG22	10	0.42
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG23	10	0.42
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	5	0.42
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	5	0.42
(1,1214)	1:B:274:LEU:HD11	1:A:237:ARG:HD3	8	0.42
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	18	0.42
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	18	0.42
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	18	0.42
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	17	0.41
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	18	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG22	8	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG21	8	0.41
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG23	8	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD12	8	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD11	8	0.41
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD13	8	0.41
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG22	8	0.41
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG21	8	0.41
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG23	8	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD12	8	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD11	8	0.41
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD13	8	0.41
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	19	0.41
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	19	0.41
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	19	0.41
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	19	0.41
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	16	0.41
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	16	0.41
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	16	0.41
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	5	0.41
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	1	0.41
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	3	0.41
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	12	0.41
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	3	0.41
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	12	0.41
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	11	0.41
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	3	0.41
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	2	0.41
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	12	0.41
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	12	0.41
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	12	0.41
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	8	0.41
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	8	0.41
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	19	0.41
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	14	0.41
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	15	0.4
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	15	0.4
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	16	0.4
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	16	0.4
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	16	0.4
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	8	0.4
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	8	0.4
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	8	0.4
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	16	0.4
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	9	0.4
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	9	0.4
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	20	0.4
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	20	0.4
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	15	0.4
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	15	0.4
(1,3449)	1:A:239:SER:H	1:A:260:ILE:HG13	9	0.4
(1,3449)	1:A:239:SER:H	1:B:274:LEU:HG	9	0.4
(1,3449)	1:A:239:SER:H	1:B:280:ARG:HB2	9	0.4
(1,310)	1:B:260:ILE:HD11	1:A:262:ILE:HG12	3	0.4
(1,309)	1:A:260:ILE:HD11	1:B:262:ILE:HG12	3	0.4
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	2	0.4
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	9	0.4
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	16	0.4
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	2	0.4
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	9	0.4
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	16	0.4
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	11	0.4
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG21	10	0.4
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG22	10	0.4
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG23	10	0.4
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	2	0.4
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	19	0.4
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	19	0.4
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	17	0.4
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	17	0.4
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	17	0.4
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	17	0.4
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	17	0.4
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	17	0.4
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	12	0.4
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	12	0.4
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	11	0.4
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	16	0.39
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	4	0.39
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	8	0.39
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	8	0.39
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	8	0.39
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	5	0.39
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	5	0.39
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	18	0.39
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	14	0.39
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	14	0.39
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	20	0.39
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	20	0.39
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	15	0.39
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	15	0.39
(1,3450)	1:B:239:SER:H	1:B:260:ILE:HG13	9	0.39
(1,3450)	1:B:239:SER:H	1:A:274:LEU:HG	9	0.39
(1,3450)	1:B:239:SER:H	1:A:280:ARG:HB2	9	0.39
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	3	0.39
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	3	0.39
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	8	0.39
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	8	0.39
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	8	0.39
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	8	0.39
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	5	0.39
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	6	0.39
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	6	0.39
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	10	0.39
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD22	5	0.39
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD21	5	0.39
(1,1270)	1:B:253:ARG:HD2	1:B:234:LEU:HD23	5	0.39
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD22	5	0.39
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD21	5	0.39
(1,1269)	1:A:253:ARG:HD2	1:A:234:LEU:HD23	5	0.39
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	20	0.39
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	6	0.39
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	6	0.39
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	6	0.39
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	16	0.38
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	16	0.38
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	16	0.38
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	4	0.38
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	15	0.38
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	4	0.38
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	15	0.38
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	17	0.38
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	17	0.38
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	17	0.38
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	17	0.38
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	20	0.38
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	20	0.38
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	20	0.38
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	20	0.38
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	16	0.38
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	16	0.38
(1,3291)	1:A:233:VAL:HG22	1:A:230:LYS:HB3	1	0.38
(1,3291)	1:A:233:VAL:HG21	1:A:230:LYS:HB3	1	0.38
(1,3291)	1:A:233:VAL:HG23	1:A:230:LYS:HB3	1	0.38
(1,3291)	1:A:249:VAL:HG22	1:B:277:LEU:HB3	1	0.38
(1,3291)	1:A:249:VAL:HG21	1:B:277:LEU:HB3	1	0.38
(1,3291)	1:A:249:VAL:HG23	1:B:277:LEU:HB3	1	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	9	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	9	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	16	0.38
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	16	0.38
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	9	0.38
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	9	0.38
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	16	0.38
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	16	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG22	7	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG21	7	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG23	7	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD12	7	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD11	7	0.38
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD13	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG22	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG21	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG23	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD12	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD11	7	0.38
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD13	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	15	0.38
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	15	0.38
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	15	0.38
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	15	0.38
(1,2092)	1:B:257:LYS:H	1:B:257:LYS:HB3	15	0.38
(1,2091)	1:A:257:LYS:H	1:A:257:LYS:HB3	15	0.38
(1,2076)	1:B:257:LYS:H	1:B:255:LYS:HB3	5	0.38
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	10	0.38
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	11	0.38
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	11	0.38
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	11	0.38
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	11	0.38
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	11	0.38
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	11	0.38
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	20	0.38
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	5	0.37
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	7	0.37
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	7	0.37
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	17	0.37
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	17	0.37
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	17	0.37
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	17	0.37
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	8	0.37
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	17	0.37
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	17	0.37
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	17	0.37
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	17	0.37
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	16	0.37
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	16	0.37
(1,3292)	1:B:233:VAL:HG22	1:B:230:LYS:HB3	1	0.37
(1,3292)	1:B:233:VAL:HG21	1:B:230:LYS:HB3	1	0.37
(1,3292)	1:B:233:VAL:HG23	1:B:230:LYS:HB3	1	0.37
(1,3292)	1:B:249:VAL:HG22	1:A:277:LEU:HB3	1	0.37
(1,3292)	1:B:249:VAL:HG21	1:A:277:LEU:HB3	1	0.37
(1,3292)	1:B:249:VAL:HG23	1:A:277:LEU:HB3	1	0.37
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	5	0.37
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	5	0.37
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	5	0.37
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	5	0.37
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	5	0.37
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	5	0.37
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	17	0.37
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	17	0.37
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	17	0.37
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	6	0.37
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	9	0.37
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	9	0.37
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	15	0.37
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	15	0.37
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	15	0.37
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	15	0.37
(1,2075)	1:A:257:LYS:H	1:A:255:LYS:HB3	5	0.37
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	3	0.37
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	3	0.37
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	20	0.37
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	7	0.37
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	6	0.37
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	6	0.37
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	6	0.37
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	5	0.36
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	13	0.36
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	2	0.36
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	2	0.36
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	2	0.36
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	8	0.36
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	8	0.36
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	8	0.36
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	8	0.36
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	8	0.36
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	6	0.36
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	6	0.36
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG22	20	0.36
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG21	20	0.36
(1,3520)	1:B:247:THR:H	1:B:273:ILE:HG23	20	0.36
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD12	20	0.36
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD11	20	0.36
(1,3520)	1:B:247:THR:H	1:B:276:LEU:HD13	20	0.36
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG22	20	0.36
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG21	20	0.36
(1,3519)	1:A:247:THR:H	1:A:273:ILE:HG23	20	0.36
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD12	20	0.36
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD11	20	0.36
(1,3519)	1:A:247:THR:H	1:A:276:LEU:HD13	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	15	0.36
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	15	0.36
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD22	6	0.36
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD21	6	0.36
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD23	6	0.36
(1,2352)	1:B:266:SER:H	1:B:264:PHE:HD2	15	0.36
(1,2351)	1:A:266:SER:H	1:A:264:PHE:HD2	15	0.36
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	11	0.36
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	15	0.36
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	15	0.36
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG21	14	0.36
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG22	14	0.36
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG23	14	0.36
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	19	0.36
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	15	0.36
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	15	0.36
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	15	0.36
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	15	0.36
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	15	0.36
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	15	0.36
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	14	0.36
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	1	0.36
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	8	0.36
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	8	0.36
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	8	0.36
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	8	0.36
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	16	0.35
(2,26)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	8	0.35
(2,25)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	8	0.35
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	13	0.35
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	3	0.35
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	3	0.35
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	3	0.35
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	3	0.35
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	19	0.35
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	19	0.35
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	19	0.35
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	6	0.35
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	6	0.35
(1,2684)	1:B:281:GLU:H	1:B:281:GLU:HG3	9	0.35
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	11	0.35
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	5	0.35
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	5	0.35
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	13	0.35
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	13	0.35
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG21	14	0.35
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG22	14	0.35
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG23	14	0.35
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	19	0.35
(1,1172)	1:B:276:LEU:H	1:B:276:LEU:HD21	10	0.35
(1,1171)	1:A:276:LEU:H	1:A:276:LEU:HD21	10	0.35
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	8	0.35
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	8	0.35
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	8	0.35
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	8	0.35
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	19	0.34
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	19	0.34
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	3	0.34
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	3	0.34
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	18	0.34
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	16	0.34
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	16	0.34
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	16	0.34
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	16	0.34
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	4	0.34
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	13	0.34
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	4	0.34
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	13	0.34
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	2	0.34
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	2	0.34
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	2	0.34
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	14	0.34
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	14	0.34
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	1	0.34
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	1	0.34
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	8	0.34
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	8	0.34
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	9	0.34
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	3	0.34
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	18	0.34
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	3	0.34
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	18	0.34
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	20	0.34
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	20	0.34
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	20	0.34
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	8	0.34
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	8	0.34
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	8	0.34
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	8	0.34
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	1	0.34
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	1	0.34
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	10	0.34
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	10	0.34
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	10	0.34
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	10	0.34
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	5	0.34
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	5	0.34
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	5	0.34
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	5	0.34
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	14	0.34
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	14	0.34
(1,3068)	1:B:251:ILE:HD11	1:B:234:LEU:HB3	5	0.34
(1,3068)	1:B:251:ILE:HD11	1:B:251:ILE:HB	5	0.34
(1,3067)	1:A:251:ILE:HD11	1:A:234:LEU:HB3	5	0.34
(1,3067)	1:A:251:ILE:HD11	1:A:251:ILE:HB	5	0.34
(1,2683)	1:A:281:GLU:H	1:A:281:GLU:HG3	9	0.34
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	6	0.34
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD22	6	0.34
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD21	6	0.34
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD23	6	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	5	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	5	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	5	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	11	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	11	0.34
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	11	0.34
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	11	0.34
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	11	0.34
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	11	0.34
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD12	8	0.34
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD11	8	0.34
(1,1974)	1:B:253:ARG:H	1:B:234:LEU:HD13	8	0.34
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	1	0.34
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	12	0.33
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	16	0.33
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	6	0.33
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	6	0.33
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	18	0.33
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	13	0.33
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	13	0.33
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	3	0.33
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	17	0.33
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	3	0.33
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	9	0.33
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	15	0.33
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	15	0.33
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	15	0.33
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	12	0.33
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	12	0.33
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	12	0.33
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	15	0.33
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	15	0.33
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	15	0.33
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	5	0.33
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	5	0.33
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	5	0.33
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	5	0.33
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	9	0.33
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	9	0.33
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	9	0.33
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	11	0.33
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD12	8	0.33
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD11	8	0.33
(1,1973)	1:A:253:ARG:H	1:A:234:LEU:HD13	8	0.33
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	4	0.33
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	4	0.33
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	14	0.33
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	14	0.33
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	7	0.33
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	16	0.33
(3,10)	1:A:251:ILE:H	1:A:238:GLU:OE1	6	0.32
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	12	0.32
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	13	0.32
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	13	0.32
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	3	0.32
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	17	0.32
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	15	0.32
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	8	0.32
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	8	0.32
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	17	0.32
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	12	0.32
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	12	0.32
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	12	0.32
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	14	0.32
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	14	0.32
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	18	0.32
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	18	0.32
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	17	0.32
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	17	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	7	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	7	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	7	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	9	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	9	0.32
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	9	0.32
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	6	0.32
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	11	0.32
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	17	0.32
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	9	0.32
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	9	0.32
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	2	0.31
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	2	0.31
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	16	0.31
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	3	0.31
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	14	0.31
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	14	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	11	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	11	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	11	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	13	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	13	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	13	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	19	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	19	0.31
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	19	0.31
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	14	0.31
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	12	0.31
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	5	0.31
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	5	0.31
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	18	0.31
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	18	0.31
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	18	0.31
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	18	0.31
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	18	0.31
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	18	0.31
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	2	0.31
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	2	0.31
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	2	0.31
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	19	0.31
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	19	0.31
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	19	0.31
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	2	0.31
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	2	0.31
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	2	0.31
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	19	0.31
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	19	0.31
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	19	0.31
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	2	0.31
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	2	0.31
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	2	0.31
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	2	0.31
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	2	0.31
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	2	0.31
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	6	0.31
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	18	0.31
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	17	0.31
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	9	0.31
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	13	0.31
(3,34)	1:B:251:ILE:H	1:B:238:GLU:OE1	6	0.3
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	17	0.3
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	16	0.3
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	5	0.3
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	8	0.3
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	16	0.3
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	8	0.3
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	11	0.3
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	13	0.3
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	13	0.3
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	13	0.3
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	15	0.3
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	14	0.3
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	12	0.3
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	1	0.3
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	1	0.3
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	6	0.3
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	15	0.3
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	1	0.3
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	6	0.3
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	11	0.3
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	5	0.3
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	5	0.3
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	6	0.3
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	6	0.3
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	7	0.3
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	7	0.3
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	7	0.3
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	7	0.3
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	16	0.3
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	16	0.3
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	16	0.3
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	7	0.3
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	7	0.3
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	7	0.3
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	7	0.3
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	2	0.3
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	2	0.3
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	2	0.3
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	2	0.3
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	2	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	2	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	2	0.3
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	2	0.3
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	15	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	15	0.3
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	15	0.3
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	15	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	7	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	7	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	16	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	16	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	16	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	20	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	20	0.3
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	20	0.3
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	12	0.3
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	12	0.3
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	18	0.3
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	13	0.3
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	13	0.3
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	14	0.3
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	14	0.3
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	7	0.3
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	7	0.3
(1,1162)	1:B:251:ILE:HD11	1:A:264:PHE:HZ	18	0.3
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	5	0.29
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	7	0.29
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	7	0.29
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	6	0.29
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	11	0.29
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	5	0.29
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	6	0.29
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	12	0.29
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	11	0.29
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	15	0.29
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	1	0.29
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	1	0.29
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	1	0.29
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	1	0.29
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	3	0.29
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	3	0.29
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	3	0.29
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	3	0.29
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	1	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	1	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	1	0.29
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	1	0.29
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	3	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	3	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	3	0.29
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	15	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	15	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	15	0.29
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	15	0.29
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	16	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	16	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	16	0.29
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	16	0.29
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	19	0.29
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	19	0.29
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	19	0.29
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	19	0.29
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	6	0.29
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	6	0.29
(1,3739)	1:A:270:LEU:H	1:A:274:LEU:HB3	11	0.29
(1,3739)	1:A:270:LEU:H	1:B:253:ARG:HB3	11	0.29
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	6	0.29
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	6	0.29
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	6	0.29
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	16	0.29
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	16	0.29
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	16	0.29
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	6	0.29
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	6	0.29
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	6	0.29
(1,330)	1:B:251:ILE:HD11	1:B:238:GLU:HG2	4	0.29
(1,329)	1:A:251:ILE:HD11	1:A:238:GLU:HG2	4	0.29
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	15	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	15	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	15	0.29
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	15	0.29
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	18	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	18	0.29
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	18	0.29
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	18	0.29
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	18	0.29
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	18	0.29
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	18	0.29
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	18	0.29
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	15	0.29
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	15	0.29
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	15	0.29
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	11	0.29
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	11	0.29
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	9	0.29
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	9	0.29
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	9	0.29
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	6	0.29
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	6	0.29
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	16	0.29
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	16	0.29
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	16	0.29
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	16	0.29
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	20	0.29
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	20	0.29
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	20	0.29
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	16	0.29
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	16	0.29
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	9	0.29
(1,1162)	1:B:251:ILE:HD11	1:A:264:PHE:HZ	10	0.29
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	13	0.29
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	17	0.28
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	19	0.28
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	8	0.28
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	12	0.28
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	8	0.28
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	12	0.28
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	19	0.28
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	11	0.28
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	11	0.28
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	11	0.28
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	11	0.28
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	11	0.28
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	12	0.28
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	1	0.28
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	12	0.28
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	16	0.28
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	15	0.28
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	15	0.28
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	15	0.28
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	15	0.28
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	13	0.28
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	13	0.28
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	13	0.28
(1,3740)	1:B:270:LEU:H	1:B:274:LEU:HB3	11	0.28
(1,3740)	1:B:270:LEU:H	1:A:253:ARG:HB3	11	0.28
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	7	0.28
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	7	0.28
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	7	0.28
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	7	0.28
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	7	0.28
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	7	0.28
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	11	0.28
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	11	0.28
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	7	0.28
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	7	0.28
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	7	0.28
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	9	0.28
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	9	0.28
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	9	0.28
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	7	0.28
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	7	0.28
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	7	0.28
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	9	0.28
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	9	0.28
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	9	0.28
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	9	0.28
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	9	0.28
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	9	0.28
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	12	0.28
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	16	0.28
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	12	0.28
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	20	0.28
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	20	0.28
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	20	0.28
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	16	0.28
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	13	0.28
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	13	0.28
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD22	8	0.28
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD21	8	0.28
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD23	8	0.28
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD22	8	0.28
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD21	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD23	8	0.28
(1,1412)	1:B:234:LEU:H	1:B:233:VAL:HG21	7	0.28
(1,1411)	1:A:234:LEU:H	1:A:233:VAL:HG21	7	0.28
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	3	0.28
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	5	0.27
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	8	0.27
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	1	0.27
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	19	0.27
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	1	0.27
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	14	0.27
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	14	0.27
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	14	0.27
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	18	0.27
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	18	0.27
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	18	0.27
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	5	0.27
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	5	0.27
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD12	9	0.27
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD11	9	0.27
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD13	9	0.27
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD12	9	0.27
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD11	9	0.27
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD13	9	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	5	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	5	0.27
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	5	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	11	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	11	0.27
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	11	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	19	0.27
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	19	0.27
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	19	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	5	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	5	0.27
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	5	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	11	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	11	0.27
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	11	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	19	0.27
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	19	0.27
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	19	0.27
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	13	0.27
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	13	0.27
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	13	0.27
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	13	0.27
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	13	0.27
(1,304)	1:B:260:ILE:H	1:B:260:ILE:HD11	4	0.27
(1,303)	1:A:260:ILE:H	1:A:260:ILE:HD11	4	0.27
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	16	0.27
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	19	0.27
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	19	0.27
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	19	0.27
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	20	0.27
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	20	0.27
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	15	0.27
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	15	0.27
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	5	0.27
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	5	0.27
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	5	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	5	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	5	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	5	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	20	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	20	0.27
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	20	0.27
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	14	0.27
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	14	0.27
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	14	0.27
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	14	0.27
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	14	0.27
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	14	0.27
(1,1161)	1:A:251:ILE:HD11	1:B:264:PHE:HZ	18	0.27
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	3	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	3	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	7	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	8	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	11	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	12	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	13	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	14	0.27
(1,110)	1:B:229:VAL:HA	1:B:229:VAL:HB	16	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	3	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	8	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	11	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	12	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	13	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	14	0.27
(1,109)	1:A:229:VAL:HA	1:A:229:VAL:HB	16	0.27
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	12	0.27
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	18	0.26
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	18	0.26
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	8	0.26
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	3	0.26
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	3	0.26
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	3	0.26
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	14	0.26
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	14	0.26
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	10	0.26
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	17	0.26
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	17	0.26
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	17	0.26
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	17	0.26
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	17	0.26
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	3	0.26
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	3	0.26
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	3	0.26
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	8	0.26
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	8	0.26
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	8	0.26
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	3	0.26
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	3	0.26
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	3	0.26
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	8	0.26
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	8	0.26
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	8	0.26
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	10	0.26
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	10	0.26
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	10	0.26
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	10	0.26
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	17	0.26
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	17	0.26
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	17	0.26
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	17	0.26
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	17	0.26
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	14	0.26
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	14	0.26
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	18	0.26
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	18	0.26
(1,1334)	1:B:266:SER:H	1:A:256:LYS:HA	6	0.26
(1,1161)	1:A:251:ILE:HD11	1:B:264:PHE:HZ	10	0.26
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	20	0.26
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	12	0.26
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	20	0.26
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	3	0.25
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	3	0.25
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	3	0.25
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	14	0.25
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	14	0.25
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	15	0.25
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	9	0.25
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	9	0.25
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	9	0.25
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	16	0.25
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	16	0.25
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	16	0.25
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	16	0.25
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	19	0.25
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	19	0.25
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	19	0.25
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	19	0.25
(1,364)	1:B:262:ILE:HG21	1:B:245:PHE:HB3	3	0.25
(1,363)	1:A:262:ILE:HG21	1:A:245:PHE:HB3	3	0.25
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	13	0.25
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	13	0.25
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	13	0.25
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	13	0.25
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	13	0.25
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	13	0.25
(1,3292)	1:B:233:VAL:HG22	1:B:230:LYS:HB3	19	0.25
(1,3292)	1:B:233:VAL:HG21	1:B:230:LYS:HB3	19	0.25
(1,3292)	1:B:233:VAL:HG23	1:B:230:LYS:HB3	19	0.25
(1,3292)	1:B:249:VAL:HG22	1:A:277:LEU:HB3	19	0.25
(1,3292)	1:B:249:VAL:HG21	1:A:277:LEU:HB3	19	0.25
(1,3292)	1:B:249:VAL:HG23	1:A:277:LEU:HB3	19	0.25
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	1	0.25
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	4	0.25
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	4	0.25
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	6	0.25
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	6	0.25
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	6	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	6	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	6	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	6	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	19	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	19	0.25
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	19	0.25
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	6	0.25
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	11	0.25
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	6	0.25
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	11	0.25
(1,1700)	1:B:243:ASN:HD22	1:B:243:ASN:HB3	17	0.25
(1,1699)	1:A:243:ASN:HD22	1:A:243:ASN:HB3	17	0.25
(1,1699)	1:A:243:ASN:HD22	1:A:243:ASN:HB3	20	0.25
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	9	0.25
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	9	0.25
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	12	0.25
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	5	0.25
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	5	0.25
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	5	0.25
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	16	0.25
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	16	0.25
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	16	0.25
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	5	0.25
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	5	0.25
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	5	0.25
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	16	0.25
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	16	0.25
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	16	0.25
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	12	0.25
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	12	0.25
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	14	0.25
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	14	0.25
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	14	0.25
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	7	0.25
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	15	0.24
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	15	0.24
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	16	0.24
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	5	0.24
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	5	0.24
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	5	0.24
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	4	0.24
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	4	0.24
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	4	0.24
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	4	0.24
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	12	0.24
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	15	0.24
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	12	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	6	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	6	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	6	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	18	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	18	0.24
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	18	0.24
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	10	0.24
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	5	0.24
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	5	0.24
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	16	0.24
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	16	0.24
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	3	0.24
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	16	0.24
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	3	0.24
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD22	4	0.24
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD21	4	0.24
(1,400)	1:B:251:ILE:HG21	1:A:270:LEU:HD23	4	0.24
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD22	4	0.24
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD21	4	0.24
(1,399)	1:A:251:ILE:HG21	1:B:270:LEU:HD23	4	0.24
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	4	0.24
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	4	0.24
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	7	0.24
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	7	0.24
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	7	0.24
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	7	0.24
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	10	0.24
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	10	0.24
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	10	0.24
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	2	0.24
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	2	0.24
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	3	0.24
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	3	0.24
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE2	9	0.24
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE3	9	0.24
(1,3341)	1:A:251:ILE:HG21	1:B:264:PHE:HB3	9	0.24
(1,3291)	1:A:233:VAL:HG22	1:A:230:LYS:HB3	19	0.24
(1,3291)	1:A:233:VAL:HG21	1:A:230:LYS:HB3	19	0.24
(1,3291)	1:A:233:VAL:HG23	1:A:230:LYS:HB3	19	0.24
(1,3291)	1:A:249:VAL:HG22	1:B:277:LEU:HB3	19	0.24
(1,3291)	1:A:249:VAL:HG21	1:B:277:LEU:HB3	19	0.24
(1,3291)	1:A:249:VAL:HG23	1:B:277:LEU:HB3	19	0.24
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	15	0.24
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	15	0.24
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	15	0.24
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	15	0.24
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	15	0.24
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	15	0.24
(1,3098)	1:B:231:ASP:HB3	1:B:254:GLN:HE22	16	0.24
(1,3098)	1:B:231:ASP:HB2	1:B:257:LYS:H	16	0.24
(1,3098)	1:B:231:ASP:HB2	1:B:254:GLN:HE22	16	0.24
(1,3098)	1:B:231:ASP:HB3	1:B:257:LYS:H	16	0.24
(1,3097)	1:A:231:ASP:HB3	1:A:254:GLN:HE22	16	0.24
(1,3097)	1:A:231:ASP:HB2	1:A:257:LYS:H	16	0.24
(1,3097)	1:A:231:ASP:HB2	1:A:254:GLN:HE22	16	0.24
(1,3097)	1:A:231:ASP:HB3	1:A:257:LYS:H	16	0.24
(1,1700)	1:B:243:ASN:HD22	1:B:243:ASN:HB3	11	0.24
(1,1700)	1:B:243:ASN:HD22	1:B:243:ASN:HB3	15	0.24
(1,1700)	1:B:243:ASN:HD22	1:B:243:ASN:HB3	20	0.24
(1,1699)	1:A:243:ASN:HD22	1:A:243:ASN:HB3	11	0.24
(1,1699)	1:A:243:ASN:HD22	1:A:243:ASN:HB3	15	0.24
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	11	0.24
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	11	0.24
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	11	0.24
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	11	0.24
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	11	0.24
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	11	0.24
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	12	0.24
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	8	0.24
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	14	0.24
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	14	0.24
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	7	0.24
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	14	0.24
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	16	0.24
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	2	0.24
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	14	0.24
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	16	0.24
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB2	9	0.24
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB3	9	0.24
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB2	9	0.24
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB3	9	0.24
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	16	0.23
(3,46)	1:B:277:LEU:H	1:B:273:ILE:O	9	0.23
(3,22)	1:A:277:LEU:H	1:A:273:ILE:O	9	0.23
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	5	0.23
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	5	0.23
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	5	0.23
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	1	0.23
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	1	0.23
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	1	0.23
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	1	0.23
(1,852)	1:B:235:LYS:HG2	1:B:236:GLU:HA	4	0.23
(1,852)	1:B:235:LYS:HG3	1:B:236:GLU:HA	4	0.23
(1,851)	1:A:235:LYS:HG2	1:A:236:GLU:HA	4	0.23
(1,851)	1:A:235:LYS:HG3	1:A:236:GLU:HA	4	0.23
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	9	0.23
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	9	0.23
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	9	0.23
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	17	0.23
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	19	0.23
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	19	0.23
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	3	0.23
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	3	0.23
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	2	0.23
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	2	0.23
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	2	0.23
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE2	9	0.23
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE3	9	0.23
(1,3342)	1:B:251:ILE:HG21	1:A:264:PHE:HB3	9	0.23
(1,3228)	1:B:276:LEU:HD21	1:B:275:GLU:HB2	10	0.23
(1,3228)	1:B:276:LEU:HD21	1:B:275:GLU:HB3	10	0.23
(1,3228)	1:B:276:LEU:HB3	1:B:276:LEU:HD21	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3227)	1:A:276:LEU:HD21	1:A:275:GLU:HB2	10	0.23
(1,3227)	1:A:276:LEU:HD21	1:A:275:GLU:HB3	10	0.23
(1,3227)	1:A:276:LEU:HB3	1:A:276:LEU:HD21	10	0.23
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	14	0.23
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	14	0.23
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	14	0.23
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	14	0.23
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	14	0.23
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	14	0.23
(1,2945)	1:A:272:ARG:HE	1:A:269:ASP:HA	13	0.23
(1,2663)	1:A:280:ARG:H	1:A:281:GLU:HG3	7	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD22	20	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD21	20	0.23
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD23	20	0.23
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD22	1	0.23
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD21	1	0.23
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD23	1	0.23
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	19	0.23
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	19	0.23
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	19	0.23
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	19	0.23
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	19	0.23
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	19	0.23
(1,1044)	1:B:234:LEU:HB3	1:A:270:LEU:HD11	2	0.23
(1,1043)	1:A:234:LEU:HB3	1:B:270:LEU:HD11	2	0.23
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	2	0.23
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	8	0.22
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	14	0.22
(1,898)	1:B:237:ARG:H	1:B:241:LEU:HD21	10	0.22
(1,897)	1:A:237:ARG:H	1:A:241:LEU:HD21	10	0.22
(1,882)	1:B:252:LYS:HG3	1:B:252:LYS:HE2	7	0.22
(1,881)	1:A:252:LYS:HG3	1:A:252:LYS:HE2	7	0.22
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	20	0.22
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	20	0.22
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	20	0.22
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	3	0.22
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	19	0.22
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	3	0.22
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	3	0.22
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	3	0.22
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	3	0.22
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	2	0.22
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	2	0.22
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	2	0.22
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	2	0.22
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE2	16	0.22
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE3	16	0.22
(1,3342)	1:B:251:ILE:HG21	1:A:264:PHE:HB3	16	0.22
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE2	16	0.22
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE3	16	0.22
(1,3341)	1:A:251:ILE:HG21	1:B:264:PHE:HB3	16	0.22
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	3	0.22
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	3	0.22
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	3	0.22
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	3	0.22
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	3	0.22
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	3	0.22
(1,2946)	1:B:272:ARG:HE	1:B:269:ASP:HA	13	0.22
(1,2664)	1:B:280:ARG:H	1:B:281:GLU:HG3	7	0.22
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD22	14	0.22
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD21	14	0.22
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD23	14	0.22
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	7	0.22
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	7	0.22
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD22	18	0.22
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD21	18	0.22
(1,2172)	1:B:260:ILE:H	1:A:270:LEU:HD23	18	0.22
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD22	18	0.22
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD21	18	0.22
(1,2171)	1:A:260:ILE:H	1:B:270:LEU:HD23	18	0.22
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	3	0.22
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	19	0.22
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	3	0.22
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	19	0.22
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	12	0.22
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	12	0.22
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	7	0.22
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	7	0.22
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	12	0.22
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	12	0.22
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD22	1	0.22
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD21	1	0.22
(1,1724)	1:B:245:PHE:H	1:B:276:LEU:HD23	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD22	20	0.22
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD21	20	0.22
(1,1723)	1:A:245:PHE:H	1:A:276:LEU:HD23	20	0.22
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	15	0.22
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	15	0.22
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	13	0.22
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	13	0.22
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	13	0.22
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	13	0.22
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	13	0.22
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	13	0.22
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	8	0.22
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	3	0.22
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	8	0.22
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	3	0.22
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	8	0.22
(3,39)	1:B:266:SER:H	1:B:269:ASP:OD1	7	0.21
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	14	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	1	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	1	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	1	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	10	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	10	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	10	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	12	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	12	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	12	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	16	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	16	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	16	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	19	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	19	0.21
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	19	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	1	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	1	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	1	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	10	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	10	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	10	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	12	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	12	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	16	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	16	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	16	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	19	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	19	0.21
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	19	0.21
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	14	0.21
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	14	0.21
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	14	0.21
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	19	0.21
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	20	0.21
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	3	0.21
(1,387)	1:A:252:LYS:H	1:A:251:ILE:HG21	7	0.21
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	7	0.21
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	7	0.21
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	7	0.21
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	7	0.21
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	10	0.21
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	10	0.21
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	10	0.21
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	10	0.21
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	10	0.21
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	10	0.21
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	20	0.21
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	20	0.21
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	20	0.21
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	20	0.21
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	20	0.21
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	20	0.21
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	11	0.21
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	13	0.21
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	13	0.21
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD22	14	0.21
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD21	14	0.21
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD23	14	0.21
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	1	0.21
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	1	0.21
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	3	0.21
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	19	0.21
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG21	16	0.21
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG22	16	0.21
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG23	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1786)	1:B:247:THR:H	1:B:262:ILE:HG21	11	0.21
(1,1785)	1:A:247:THR:H	1:A:262:ILE:HG21	11	0.21
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	14	0.21
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	20	0.21
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	14	0.21
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	16	0.21
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	20	0.21
(1,1333)	1:A:266:SER:H	1:B:256:LYS:HA	6	0.21
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	2	0.21
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	2	0.21
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	2	0.21
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	20	0.21
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	15	0.21
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	17	0.21
(1,986)	1:B:247:THR:HG21	1:B:272:ARG:HE	6	0.2
(1,985)	1:A:247:THR:HG21	1:A:272:ARG:HE	6	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	8	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	8	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	8	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	20	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	20	0.2
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	20	0.2
(1,898)	1:B:237:ARG:H	1:B:241:LEU:HD21	20	0.2
(1,897)	1:A:237:ARG:H	1:A:241:LEU:HD21	20	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	20	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	20	0.2
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	20	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	5	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	5	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	5	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	6	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	6	0.2
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	6	0.2
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	19	0.2
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	19	0.2
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	19	0.2
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	8	0.2
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	5	0.2
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	18	0.2
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	14	0.2
(1,388)	1:B:252:LYS:H	1:B:251:ILE:HG21	7	0.2
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	10	0.2
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	2	0.2
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	2	0.2
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	13	0.2
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	13	0.2
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	13	0.2
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	13	0.2
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	3	0.2
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	3	0.2
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	3	0.2
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	3	0.2
(1,3278)	1:B:274:LEU:HD11	1:A:238:GLU:HG2	13	0.2
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB2	13	0.2
(1,3278)	1:B:274:LEU:HD11	1:B:275:GLU:HB3	13	0.2
(1,3278)	1:B:276:LEU:HB3	1:B:274:LEU:HD11	13	0.2
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	1	0.2
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	1	0.2
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	1	0.2
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	1	0.2
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	18	0.2
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	18	0.2
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	18	0.2
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	18	0.2
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	18	0.2
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	18	0.2
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	11	0.2
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	3	0.2
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	3	0.2
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	3	0.2
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	11	0.2
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	2	0.2
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG21	16	0.2
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG22	16	0.2
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG23	16	0.2
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	16	0.2
(1,1412)	1:B:234:LEU:H	1:B:233:VAL:HG21	18	0.2
(1,1411)	1:A:234:LEU:H	1:A:233:VAL:HG21	18	0.2
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	2	0.2
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	2	0.2
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	2	0.2
(1,1268)	1:B:253:ARG:HD3	1:B:234:LEU:HD12	17	0.2
(1,1268)	1:B:253:ARG:HD3	1:B:234:LEU:HD11	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1268)	1:B:253:ARG:HD3	1:B:234:LEU:HD13	17	0.2
(1,1267)	1:A:253:ARG:HD3	1:A:234:LEU:HD12	17	0.2
(1,1267)	1:A:253:ARG:HD3	1:A:234:LEU:HD11	17	0.2
(1,1267)	1:A:253:ARG:HD3	1:A:234:LEU:HD13	17	0.2
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	15	0.2
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	17	0.19
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	11	0.19
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	17	0.19
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	8	0.19
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	5	0.19
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	6	0.19
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	6	0.19
(1,963)	1:A:242:GLN:HE22	1:A:249:VAL:HG11	5	0.19
(1,913)	1:A:241:LEU:HD21	1:B:278:SER:HA	10	0.19
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	15	0.19
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	15	0.19
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	15	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	8	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	8	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	8	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	15	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	15	0.19
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	15	0.19
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	20	0.19
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	20	0.19
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	20	0.19
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	20	0.19
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	8	0.19
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	8	0.19
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	8	0.19
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	8	0.19
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	8	0.19
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	8	0.19
(1,364)	1:B:262:ILE:HG21	1:B:245:PHE:HB3	17	0.19
(1,363)	1:A:262:ILE:HG21	1:A:245:PHE:HB3	17	0.19
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	6	0.19
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	6	0.19
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	11	0.19
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	11	0.19
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	6	0.19
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	6	0.19
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	11	0.19
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	10	0.19
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	10	0.19
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	10	0.19
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	9	0.19
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	9	0.19
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	2	0.19
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	2	0.19
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	9	0.19
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	9	0.19
(1,3277)	1:A:274:LEU:HD11	1:B:238:GLU:HG2	13	0.19
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB2	13	0.19
(1,3277)	1:A:274:LEU:HD11	1:A:275:GLU:HB3	13	0.19
(1,3277)	1:A:276:LEU:HB3	1:A:274:LEU:HD11	13	0.19
(1,3270)	1:B:277:LEU:HD21	1:A:272:ARG:HD2	4	0.19
(1,3270)	1:B:277:LEU:HD21	1:A:245:PHE:HB3	4	0.19
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	10	0.19
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	10	0.19
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	10	0.19
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	10	0.19
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	6	0.19
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	6	0.19
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	6	0.19
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	6	0.19
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	6	0.19
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	6	0.19
(1,2340)	1:B:266:SER:H	1:B:269:ASP:HB3	20	0.19
(1,2339)	1:A:266:SER:H	1:A:269:ASP:HB3	20	0.19
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	19	0.19
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	11	0.19
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	2	0.19
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	19	0.19
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	19	0.19
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	5	0.19
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	11	0.18
(3,45)	1:B:276:LEU:H	1:B:272:ARG:O	15	0.18
(3,21)	1:A:276:LEU:H	1:A:272:ARG:O	15	0.18
(3,15)	1:A:266:SER:H	1:A:269:ASP:OD1	7	0.18
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	8	0.18
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	3	0.18
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	4	0.18
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	12	0.18
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	16	0.18
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	3	0.18
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	4	0.18
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	7	0.18
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	12	0.18
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	16	0.18
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	9	0.18
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	9	0.18
(1,964)	1:B:242:GLN:HE22	1:B:249:VAL:HG11	5	0.18
(1,964)	1:B:242:GLN:HE22	1:B:249:VAL:HG11	14	0.18
(1,963)	1:A:242:GLN:HE22	1:A:249:VAL:HG11	14	0.18
(1,407)	1:A:269:ASP:HB3	1:B:258:GLY:H	8	0.18
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	15	0.18
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD12	10	0.18
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD11	10	0.18
(1,401)	1:A:251:ILE:HG21	1:B:270:LEU:HD13	10	0.18
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	19	0.18
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	19	0.18
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	15	0.18
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	15	0.18
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	15	0.18
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	15	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	7	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	7	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	17	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	17	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	18	0.18
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	18	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	7	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	7	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	17	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	17	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	18	0.18
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	18	0.18
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	10	0.18
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	10	0.18
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	10	0.18
(1,3284)	1:B:248:THR:HG21	1:B:245:PHE:HB2	20	0.18
(1,3284)	1:B:248:THR:HG21	1:B:252:LYS:HE2	20	0.18
(1,3276)	1:B:276:LEU:HD11	1:B:272:ARG:HD2	8	0.18
(1,3276)	1:B:276:LEU:HD11	1:B:245:PHE:HB3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3275)	1:A:276:LEU:HD11	1:A:272:ARG:HD2	8	0.18
(1,3275)	1:A:276:LEU:HD11	1:A:245:PHE:HB3	8	0.18
(1,3269)	1:A:277:LEU:HD21	1:B:272:ARG:HD2	4	0.18
(1,3269)	1:A:277:LEU:HD21	1:B:245:PHE:HB3	4	0.18
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	15	0.18
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	15	0.18
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	15	0.18
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	15	0.18
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	3	0.18
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	3	0.18
(1,2690)	1:B:281:GLU:H	1:B:280:ARG:HB2	16	0.18
(1,2689)	1:A:281:GLU:H	1:A:280:ARG:HB2	16	0.18
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD22	9	0.18
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD21	9	0.18
(1,242)	1:B:253:ARG:HD2	1:A:270:LEU:HD23	9	0.18
(1,2168)	1:B:260:ILE:H	1:B:260:ILE:HD12	9	0.18
(1,2168)	1:B:260:ILE:H	1:B:260:ILE:HD11	9	0.18
(1,2168)	1:B:260:ILE:H	1:B:260:ILE:HD13	9	0.18
(1,2167)	1:A:260:ILE:H	1:A:260:ILE:HD12	9	0.18
(1,2167)	1:A:260:ILE:H	1:A:260:ILE:HD11	9	0.18
(1,2167)	1:A:260:ILE:H	1:A:260:ILE:HD13	9	0.18
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	6	0.18
(1,2114)	1:B:258:GLY:H	1:B:256:LYS:HA	17	0.18
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	6	0.18
(1,2113)	1:A:258:GLY:H	1:A:256:LYS:HA	17	0.18
(1,2090)	1:B:257:LYS:H	1:B:255:LYS:HB2	11	0.18
(1,2089)	1:A:257:LYS:H	1:A:255:LYS:HB2	11	0.18
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	13	0.18
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	13	0.18
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	6	0.18
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	11	0.18
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	11	0.18
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	11	0.18
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	15	0.18
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	18	0.18
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	15	0.18
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	18	0.18
(2,42)	1:B:270:LEU:HD21	1:A:237:ARG:HD2	3	0.17
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	16	0.17
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	16	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	1	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	5	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	8	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	9	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	10	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	11	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	13	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	14	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	15	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	18	0.17
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	19	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	1	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	2	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	5	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	8	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	9	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	10	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	13	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	14	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	15	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	18	0.17
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	19	0.17
(1,964)	1:B:242:GLN:HE22	1:B:249:VAL:HG11	11	0.17
(1,914)	1:B:241:LEU:HD21	1:A:278:SER:HA	10	0.17
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	17	0.17
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	17	0.17
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	17	0.17
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	17	0.17
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	17	0.17
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	17	0.17
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	2	0.17
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	2	0.17
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	4	0.17
(1,736)	1:B:257:LYS:HD3	1:A:265:PHE:HD2	3	0.17
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	17	0.17
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	17	0.17
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	1	0.17
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	10	0.17
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	10	0.17
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	18	0.17
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	2	0.17
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	2	0.17
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	2	0.17
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	2	0.17
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	2	0.17
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	2	0.17
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	2	0.17
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	11	0.17
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	11	0.17
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	19	0.17
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	19	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	2	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	2	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	3	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	3	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	5	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	5	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	8	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	8	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	9	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	9	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	10	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	10	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	14	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	14	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	15	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	15	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	16	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	16	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	19	0.17
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	19	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	2	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	2	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	3	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	3	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	5	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	5	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	8	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	8	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	9	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	9	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	10	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	10	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	14	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	15	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	15	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	16	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	16	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	19	0.17
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	19	0.17
(1,3283)	1:A:248:THR:HG21	1:A:245:PHE:HB2	20	0.17
(1,3283)	1:A:248:THR:HG21	1:A:252:LYS:HE2	20	0.17
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	19	0.17
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	19	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG22	18	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG21	18	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG23	18	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD12	18	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD11	18	0.17
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD13	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG22	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG21	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG23	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD12	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD11	18	0.17
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD13	18	0.17
(1,2964)	1:B:248:THR:HB	1:B:265:PHE:HD2	14	0.17
(1,2964)	1:B:248:THR:HB	1:B:245:PHE:HE2	14	0.17
(1,2963)	1:A:248:THR:HB	1:A:265:PHE:HD2	14	0.17
(1,2963)	1:A:248:THR:HB	1:A:245:PHE:HE2	14	0.17
(1,2946)	1:B:272:ARG:HE	1:B:269:ASP:HA	3	0.17
(1,2662)	1:B:280:ARG:H	1:B:279:GLU:HA	19	0.17
(1,2661)	1:A:280:ARG:H	1:A:279:GLU:HA	19	0.17
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	18	0.17
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	18	0.17
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	2	0.17
(1,2099)	1:A:257:LYS:H	1:A:257:LYS:HG2	14	0.17
(1,2052)	1:B:255:LYS:H	1:B:254:GLN:HB3	9	0.17
(1,2051)	1:A:255:LYS:H	1:A:254:GLN:HB3	9	0.17
(1,1888)	1:B:250:ASN:HD22	1:B:261:GLU:HG2	20	0.17
(1,1876)	1:B:250:ASN:HD22	1:B:252:LYS:HE2	10	0.17
(1,1830)	1:B:249:VAL:H	1:B:262:ILE:HG21	6	0.17
(1,1829)	1:A:249:VAL:H	1:A:262:ILE:HG21	6	0.17
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG21	14	0.17
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG22	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:A:242:GLN:HE21	1:A:248:THR:HG23	14	0.17
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	4	0.17
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	4	0.17
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	4	0.17
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	20	0.17
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	17	0.17
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	6	0.17
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	10	0.17
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	6	0.17
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	10	0.17
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	3	0.16
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	7	0.16
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	17	0.16
(1,972)	1:B:249:VAL:HB	1:B:249:VAL:HG11	20	0.16
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	11	0.16
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	17	0.16
(1,971)	1:A:249:VAL:HB	1:A:249:VAL:HG11	20	0.16
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	1	0.16
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	1	0.16
(1,963)	1:A:242:GLN:HE22	1:A:249:VAL:HG11	11	0.16
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	5	0.16
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	5	0.16
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	5	0.16
(1,735)	1:A:257:LYS:HD3	1:B:265:PHE:HD2	3	0.16
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	13	0.16
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	13	0.16
(1,410)	1:B:269:ASP:HB2	1:B:272:ARG:HE	12	0.16
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	1	0.16
(1,409)	1:A:269:ASP:HB2	1:A:272:ARG:HE	12	0.16
(1,408)	1:B:269:ASP:HB3	1:A:258:GLY:H	5	0.16
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	19	0.16
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	2	0.16
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD12	10	0.16
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD11	10	0.16
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD13	10	0.16
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	11	0.16
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	11	0.16
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	1	0.16
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	1	0.16
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	13	0.16
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	13	0.16
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	20	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	1	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	1	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	13	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	13	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	20	0.16
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	20	0.16
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH12	14	0.16
(1,3372)	1:B:239:SER:HA	1:B:237:ARG:HH11	14	0.16
(1,3372)	1:B:239:SER:HA	1:B:240:TYR:HE2	14	0.16
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH12	14	0.16
(1,3371)	1:A:239:SER:HA	1:A:237:ARG:HH11	14	0.16
(1,3371)	1:A:239:SER:HA	1:A:240:TYR:HE2	14	0.16
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	5	0.16
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	5	0.16
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	5	0.16
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	5	0.16
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	8	0.16
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	8	0.16
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	8	0.16
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	8	0.16
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	8	0.16
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	8	0.16
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	19	0.16
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	19	0.16
(1,2945)	1:A:272:ARG:HE	1:A:269:ASP:HA	3	0.16
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	7	0.16
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	7	0.16
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	7	0.16
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	14	0.16
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	7	0.16
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	14	0.16
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	20	0.16
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD22	9	0.16
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD21	9	0.16
(1,241)	1:A:253:ARG:HD2	1:B:270:LEU:HD23	9	0.16
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	2	0.16
(1,2100)	1:B:257:LYS:H	1:B:257:LYS:HG2	14	0.16
(1,1887)	1:A:250:ASN:HD22	1:A:261:GLU:HG2	20	0.16
(1,1774)	1:B:247:THR:H	1:B:245:PHE:HB2	11	0.16
(1,171)	1:A:274:LEU:HA	1:A:276:LEU:HB2	5	0.16
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG21	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG22	14	0.16
(1,1610)	1:B:242:GLN:HE21	1:B:248:THR:HG23	14	0.16
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	4	0.16
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	4	0.16
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	4	0.16
(1,1190)	1:B:276:LEU:HD11	1:B:245:PHE:HE1	6	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	9	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	9	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	9	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	11	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	11	0.16
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	11	0.16
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	9	0.16
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	9	0.16
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	9	0.16
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	17	0.16
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	7	0.15
(2,41)	1:A:270:LEU:HD21	1:B:237:ARG:HD2	3	0.15
(1,884)	1:B:252:LYS:HG3	1:B:250:ASN:HB2	8	0.15
(1,884)	1:B:250:ASN:HB3	1:B:252:LYS:HG3	8	0.15
(1,883)	1:A:252:LYS:HG3	1:A:250:ASN:HB2	8	0.15
(1,883)	1:A:250:ASN:HB3	1:A:252:LYS:HG3	8	0.15
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	4	0.15
(1,806)	1:B:276:LEU:HD21	1:B:273:ILE:HA	10	0.15
(1,805)	1:A:276:LEU:HD21	1:A:273:ILE:HA	10	0.15
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	11	0.15
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	14	0.15
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	15	0.15
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	9	0.15
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	9	0.15
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	9	0.15
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	9	0.15
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG12	12	0.15
(1,354)	1:B:273:ILE:HD11	1:B:273:ILE:HG13	12	0.15
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG12	12	0.15
(1,353)	1:A:273:ILE:HD11	1:A:273:ILE:HG13	12	0.15
(1,348)	1:B:272:ARG:HE	1:B:273:ILE:HD11	1	0.15
(1,347)	1:A:272:ARG:HE	1:A:273:ILE:HD11	1	0.15
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	16	0.15
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	16	0.15
(1,3282)	1:B:274:LEU:HD11	1:B:245:PHE:HE2	5	0.15
(1,3282)	1:B:274:LEU:HD11	1:A:245:PHE:HE2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3281)	1:A:274:LEU:HD11	1:A:245:PHE:HE2	5	0.15
(1,3281)	1:A:274:LEU:HD11	1:B:245:PHE:HE2	5	0.15
(1,3184)	1:B:261:GLU:HA	1:B:237:ARG:HB3	19	0.15
(1,3184)	1:B:237:ARG:HB3	1:B:250:ASN:HA	19	0.15
(1,3183)	1:A:261:GLU:HA	1:A:237:ARG:HB3	19	0.15
(1,3183)	1:A:237:ARG:HB3	1:A:250:ASN:HA	19	0.15
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	12	0.15
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	12	0.15
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	12	0.15
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	12	0.15
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	12	0.15
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	12	0.15
(1,3058)	1:B:260:ILE:HD11	1:B:234:LEU:HA	1	0.15
(1,3058)	1:B:260:ILE:HD11	1:A:275:GLU:HA	1	0.15
(1,3058)	1:B:260:ILE:HD11	1:A:248:THR:HB	1	0.15
(1,3057)	1:A:260:ILE:HD11	1:A:234:LEU:HA	1	0.15
(1,3057)	1:A:260:ILE:HD11	1:B:275:GLU:HA	1	0.15
(1,3057)	1:A:260:ILE:HD11	1:B:248:THR:HB	1	0.15
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB2	8	0.15
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB3	8	0.15
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG2	8	0.15
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG3	8	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB2	7	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB3	7	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG2	7	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG3	7	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB2	8	0.15
(1,3015)	1:A:231:ASP:HA	1:A:236:GLU:HB3	8	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG2	8	0.15
(1,3015)	1:A:231:ASP:HA	1:A:254:GLN:HG3	8	0.15
(1,2701)	1:A:282:SER:H	1:A:281:GLU:HB2	9	0.15
(1,2701)	1:A:282:SER:H	1:A:281:GLU:HB2	16	0.15
(1,2662)	1:B:280:ARG:H	1:B:279:GLU:HA	11	0.15
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	20	0.15
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	9	0.15
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	20	0.15
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	9	0.15
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	20	0.15
(1,2072)	1:B:257:LYS:H	1:B:253:ARG:HD3	1	0.15
(1,2071)	1:A:257:LYS:H	1:A:253:ARG:HD3	1	0.15
(1,1875)	1:A:250:ASN:HD22	1:A:252:LYS:HE2	10	0.15
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG21	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG22	6	0.15
(1,1872)	1:B:250:ASN:HD21	1:B:248:THR:HG23	6	0.15
(1,1773)	1:A:247:THR:H	1:A:245:PHE:HB2	11	0.15
(1,172)	1:B:274:LEU:HA	1:B:276:LEU:HB2	5	0.15
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	11	0.15
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	17	0.15
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	11	0.15
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	15	0.15
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	15	0.15
(1,1318)	1:B:260:ILE:H	1:A:270:LEU:HD11	12	0.15
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	6	0.15
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	6	0.15
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	6	0.15
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD12	18	0.15
(1,1272)	1:B:234:LEU:HD11	1:B:253:ARG:HD2	18	0.15
(1,1272)	1:B:253:ARG:HD2	1:B:234:LEU:HD13	18	0.15
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	6	0.15
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	6	0.15
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	6	0.15
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD12	18	0.15
(1,1271)	1:A:234:LEU:HD11	1:A:253:ARG:HD2	18	0.15
(1,1271)	1:A:253:ARG:HD2	1:A:234:LEU:HD13	18	0.15
(1,126)	1:B:240:TYR:HA	1:B:243:ASN:HB3	17	0.15
(1,125)	1:A:240:TYR:HA	1:A:243:ASN:HB3	17	0.15
(1,1216)	1:B:270:LEU:HD21	1:A:253:ARG:HD2	10	0.15
(1,1189)	1:A:276:LEU:HD11	1:A:245:PHE:HE1	6	0.15
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	6	0.15
(1,1151)	1:A:251:ILE:HG21	1:B:264:PHE:HZ	16	0.15
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	3	0.15
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	3	0.15
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	1	0.15
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	17	0.15
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	1	0.15
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	3	0.14
(3,6)	1:A:246:GLY:H	1:A:243:ASN:O	14	0.14
(3,46)	1:B:277:LEU:H	1:B:273:ILE:O	13	0.14
(3,30)	1:B:246:GLY:H	1:B:243:ASN:O	14	0.14
(3,22)	1:A:277:LEU:H	1:A:273:ILE:O	13	0.14
(1,999)	1:A:245:PHE:HB2	1:A:247:THR:HG21	19	0.14
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	11	0.14
(1,941)	1:A:250:ASN:HD21	1:A:248:THR:HG21	11	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	2	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	2	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	13	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	13	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	13	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD12	14	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD11	14	0.14
(1,90)	1:B:273:ILE:HA	1:B:274:LEU:HD13	14	0.14
(1,898)	1:B:237:ARG:H	1:B:241:LEU:HD21	18	0.14
(1,897)	1:A:237:ARG:H	1:A:241:LEU:HD21	18	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	2	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	2	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	2	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	14	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	14	0.14
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	14	0.14
(1,887)	1:A:234:LEU:HD11	1:A:234:LEU:HA	2	0.14
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	10	0.14
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	10	0.14
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	10	0.14
(1,751)	1:A:260:ILE:HG12	1:B:274:LEU:HG	11	0.14
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	10	0.14
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	10	0.14
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	10	0.14
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	10	0.14
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE2	7	0.14
(1,3342)	1:B:251:ILE:HG21	1:B:235:LYS:HE3	7	0.14
(1,3342)	1:B:251:ILE:HG21	1:A:264:PHE:HB3	7	0.14
(1,3302)	1:B:232:ALA:HB1	1:B:230:LYS:HB3	19	0.14
(1,3302)	1:B:232:ALA:HB1	1:B:235:LYS:HB2	19	0.14
(1,3301)	1:A:232:ALA:HB1	1:A:230:LYS:HB3	19	0.14
(1,3301)	1:A:232:ALA:HB1	1:A:235:LYS:HB2	19	0.14
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	16	0.14
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	16	0.14
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HD2	3	0.14
(1,3044)	1:B:270:LEU:HD11	1:B:264:PHE:HE2	3	0.14
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HD2	3	0.14
(1,3043)	1:A:270:LEU:HD11	1:A:264:PHE:HE2	3	0.14
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB2	7	0.14
(1,3016)	1:B:231:ASP:HA	1:B:236:GLU:HB3	7	0.14
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG2	7	0.14
(1,3016)	1:B:231:ASP:HA	1:B:254:GLN:HG3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	12	0.14
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	12	0.14
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD22	12	0.14
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD21	12	0.14
(1,2780)	1:B:244:TYR:H	1:B:276:LEU:HD23	12	0.14
(1,2702)	1:B:282:SER:H	1:B:281:GLU:HB2	9	0.14
(1,2702)	1:B:282:SER:H	1:B:281:GLU:HB2	16	0.14
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	13	0.14
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	13	0.14
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	4	0.14
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	10	0.14
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	19	0.14
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	4	0.14
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	10	0.14
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	19	0.14
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	20	0.14
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	4	0.14
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	19	0.14
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	4	0.14
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	7	0.14
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	19	0.14
(1,2352)	1:B:266:SER:H	1:B:264:PHE:HD2	18	0.14
(1,2351)	1:A:266:SER:H	1:A:264:PHE:HD2	13	0.14
(1,2351)	1:A:266:SER:H	1:A:264:PHE:HD2	18	0.14
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	20	0.14
(1,2277)	1:A:264:PHE:H	1:B:254:GLN:HB3	18	0.14
(1,2108)	1:B:257:LYS:H	1:B:254:GLN:HB3	18	0.14
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG21	6	0.14
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG22	6	0.14
(1,1871)	1:A:250:ASN:HD21	1:A:248:THR:HG23	6	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	5	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	14	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	17	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	19	0.14
(1,1626)	1:B:242:GLN:HE22	1:B:242:GLN:HG2	20	0.14
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	5	0.14
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	11	0.14
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	14	0.14
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	19	0.14
(1,1625)	1:A:242:GLN:HE22	1:A:242:GLN:HG2	20	0.14
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	11	0.14
(1,1411)	1:A:234:LEU:H	1:A:233:VAL:HG21	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:A:251:ILE:HD11	1:B:264:PHE:HE2	9	0.14
(1,1043)	1:A:234:LEU:HB3	1:B:270:LEU:HD11	9	0.14
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	5	0.14
(1,1006)	1:B:233:VAL:HA	1:B:232:ALA:HB1	11	0.14
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	5	0.14
(1,1005)	1:A:233:VAL:HA	1:A:232:ALA:HB1	11	0.14
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB2	13	0.14
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB3	13	0.14
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB2	14	0.14
(1,1001)	1:A:232:ALA:HB1	1:A:236:GLU:HB3	14	0.14
(1,1000)	1:B:245:PHE:HB2	1:B:247:THR:HG21	19	0.14
(1,922)	1:B:276:LEU:HA	1:B:276:LEU:HD11	7	0.13
(1,921)	1:A:276:LEU:HA	1:A:276:LEU:HD11	7	0.13
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD12	13	0.13
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD11	13	0.13
(1,89)	1:A:273:ILE:HA	1:A:274:LEU:HD13	13	0.13
(1,888)	1:B:234:LEU:HD11	1:B:234:LEU:HA	2	0.13
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	11	0.13
(1,406)	1:B:237:ARG:HD3	1:A:270:LEU:H	2	0.13
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG22	20	0.13
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG21	20	0.13
(1,382)	1:B:262:ILE:HG21	1:B:273:ILE:HG23	20	0.13
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG22	20	0.13
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG21	20	0.13
(1,381)	1:A:262:ILE:HG21	1:A:273:ILE:HG23	20	0.13
(1,3746)	1:B:271:ASP:H	1:B:245:PHE:HA	12	0.13
(1,3746)	1:B:271:ASP:H	1:A:230:LYS:HA	12	0.13
(1,3745)	1:A:271:ASP:H	1:A:245:PHE:HA	12	0.13
(1,3745)	1:A:271:ASP:H	1:B:230:LYS:HA	12	0.13
(1,3302)	1:B:232:ALA:HB1	1:B:230:LYS:HB3	5	0.13
(1,3302)	1:B:232:ALA:HB1	1:B:235:LYS:HB2	5	0.13
(1,3301)	1:A:232:ALA:HB1	1:A:230:LYS:HB3	5	0.13
(1,3301)	1:A:232:ALA:HB1	1:A:235:LYS:HB2	5	0.13
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	1	0.13
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	1	0.13
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	1	0.13
(1,3176)	1:B:273:ILE:HG13	1:B:263:GLU:HB3	10	0.13
(1,3176)	1:B:273:ILE:HG13	1:B:274:LEU:HB3	10	0.13
(1,3176)	1:B:273:ILE:HG13	1:A:277:LEU:HB3	10	0.13
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	1	0.13
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	1	0.13
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:A:273:ILE:HG13	1:A:263:GLU:HB3	10	0.13
(1,3175)	1:A:273:ILE:HG13	1:A:274:LEU:HB3	10	0.13
(1,3175)	1:A:273:ILE:HG13	1:B:277:LEU:HB3	10	0.13
(1,304)	1:B:260:ILE:H	1:B:260:ILE:HD11	15	0.13
(1,304)	1:B:260:ILE:H	1:B:260:ILE:HD11	18	0.13
(1,303)	1:A:260:ILE:H	1:A:260:ILE:HD11	18	0.13
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD22	12	0.13
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD21	12	0.13
(1,2779)	1:A:244:TYR:H	1:A:276:LEU:HD23	12	0.13
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	4	0.13
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	4	0.13
(1,2661)	1:A:280:ARG:H	1:A:279:GLU:HA	11	0.13
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	17	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	6	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	7	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	11	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	12	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	14	0.13
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	18	0.13
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	6	0.13
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	11	0.13
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	12	0.13
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	14	0.13
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	18	0.13
(1,2352)	1:B:266:SER:H	1:B:264:PHE:HD2	13	0.13
(1,2107)	1:A:257:LYS:H	1:A:254:GLN:HB3	18	0.13
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	19	0.13
(1,1414)	1:B:234:LEU:H	1:B:234:LEU:HD11	7	0.13
(1,1413)	1:A:234:LEU:H	1:A:234:LEU:HD11	7	0.13
(1,1412)	1:B:234:LEU:H	1:B:233:VAL:HG21	6	0.13
(1,1317)	1:A:260:ILE:H	1:B:270:LEU:HD11	12	0.13
(1,1215)	1:A:270:LEU:HD21	1:B:253:ARG:HD2	10	0.13
(1,1044)	1:B:234:LEU:HB3	1:A:270:LEU:HD11	13	0.13
(1,1043)	1:A:234:LEU:HB3	1:B:270:LEU:HD11	13	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	1	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	4	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	8	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	10	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	12	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	13	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	14	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	18	0.13
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	20	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	1	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	4	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	8	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	10	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	12	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	13	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	14	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	16	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	18	0.13
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	20	0.13
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB2	13	0.13
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB3	13	0.13
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB2	14	0.13
(1,1002)	1:B:232:ALA:HB1	1:B:236:GLU:HB3	14	0.13
(1,980)	1:B:245:PHE:H	1:B:247:THR:HG21	13	0.12
(1,979)	1:A:245:PHE:H	1:A:247:THR:HG21	13	0.12
(1,970)	1:B:249:VAL:HG11	1:B:238:GLU:HG2	2	0.12
(1,969)	1:A:249:VAL:HG11	1:A:238:GLU:HG2	2	0.12
(1,942)	1:B:250:ASN:HD21	1:B:248:THR:HG21	5	0.12
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD12	7	0.12
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD11	7	0.12
(1,837)	1:A:270:LEU:HD21	1:B:234:LEU:HD13	7	0.12
(1,752)	1:B:260:ILE:HG12	1:A:274:LEU:HG	16	0.12
(1,624)	1:B:242:GLN:HG3	1:B:262:ILE:HG13	19	0.12
(1,623)	1:A:242:GLN:HG3	1:A:262:ILE:HG13	19	0.12
(1,405)	1:A:237:ARG:HD3	1:B:270:LEU:H	20	0.12
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD12	5	0.12
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD11	5	0.12
(1,402)	1:B:251:ILE:HG21	1:A:270:LEU:HD13	5	0.12
(1,3789)	1:A:277:LEU:H	1:A:260:ILE:HB	11	0.12
(1,3789)	1:A:277:LEU:H	1:A:272:ARG:HG3	11	0.12
(1,3789)	1:A:277:LEU:H	1:B:260:ILE:HB	11	0.12
(1,3789)	1:A:277:LEU:H	1:B:251:ILE:HG12	11	0.12
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE2	7	0.12
(1,3341)	1:A:251:ILE:HG21	1:A:235:LYS:HE3	7	0.12
(1,3341)	1:A:251:ILE:HG21	1:B:264:PHE:HB3	7	0.12
(1,3314)	1:B:260:ILE:HG21	1:B:261:GLU:HB3	11	0.12
(1,3314)	1:B:260:ILE:HG21	1:B:261:GLU:HG3	11	0.12
(1,3314)	1:B:260:ILE:HG21	1:B:238:GLU:HG2	11	0.12
(1,3313)	1:A:260:ILE:HG21	1:A:261:GLU:HB3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3313)	1:A:260:ILE:HG21	1:A:261:GLU:HG3	11	0.12
(1,3313)	1:A:260:ILE:HG21	1:A:238:GLU:HG2	11	0.12
(1,303)	1:A:260:ILE:H	1:A:260:ILE:HD11	15	0.12
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	4	0.12
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	6	0.12
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	4	0.12
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	6	0.12
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	8	0.12
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	8	0.12
(1,2687)	1:A:281:GLU:H	1:A:281:GLU:HB2	15	0.12
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	2	0.12
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	5	0.12
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	6	0.12
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	8	0.12
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	17	0.12
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	2	0.12
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	5	0.12
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	8	0.12
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	5	0.12
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	16	0.12
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	5	0.12
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	16	0.12
(1,2353)	1:A:265:PHE:H	1:A:266:SER:H	15	0.12
(1,2064)	1:B:256:LYS:H	1:B:255:LYS:HB2	10	0.12
(1,2063)	1:A:256:LYS:H	1:A:255:LYS:HB2	10	0.12
(1,1825)	1:A:249:VAL:H	1:A:249:VAL:HG21	4	0.12
(1,1804)	1:B:248:THR:H	1:B:262:ILE:HG21	5	0.12
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	19	0.12
(1,1400)	1:B:234:LEU:H	1:B:234:LEU:HD21	3	0.12
(1,1399)	1:A:234:LEU:H	1:A:234:LEU:HD21	3	0.12
(1,1152)	1:B:251:ILE:HG21	1:A:264:PHE:HZ	16	0.12
(1,1044)	1:B:234:LEU:HB3	1:A:270:LEU:HD11	9	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	2	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	5	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	7	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	15	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	17	0.12
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	19	0.12
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	2	0.12
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	5	0.12
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	7	0.12
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	17	0.12
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	19	0.12
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	7	0.11
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	7	0.11
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	7	0.11
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD12	10	0.11
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD11	10	0.11
(1,838)	1:B:270:LEU:HD21	1:A:234:LEU:HD13	10	0.11
(1,812)	1:B:277:LEU:HD11	1:A:262:ILE:HD11	11	0.11
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	3	0.11
(1,811)	1:A:277:LEU:HD11	1:B:262:ILE:HD11	12	0.11
(1,420)	1:B:252:LYS:HE2	1:B:261:GLU:HG3	4	0.11
(1,419)	1:A:252:LYS:HE2	1:A:261:GLU:HG3	4	0.11
(1,397)	1:A:251:ILE:HG21	1:A:251:ILE:HB	9	0.11
(1,3790)	1:B:277:LEU:H	1:B:260:ILE:HB	11	0.11
(1,3790)	1:B:277:LEU:H	1:B:272:ARG:HG3	11	0.11
(1,3790)	1:B:277:LEU:H	1:A:260:ILE:HB	11	0.11
(1,3790)	1:B:277:LEU:H	1:A:251:ILE:HG12	11	0.11
(1,3708)	1:B:264:PHE:H	1:B:269:ASP:HA	8	0.11
(1,3708)	1:B:264:PHE:H	1:A:260:ILE:HA	8	0.11
(1,3707)	1:A:264:PHE:H	1:A:269:ASP:HA	8	0.11
(1,3707)	1:A:264:PHE:H	1:B:260:ILE:HA	8	0.11
(1,3300)	1:B:247:THR:HG21	1:B:263:GLU:HB3	11	0.11
(1,3300)	1:B:247:THR:HG21	1:A:277:LEU:HB3	11	0.11
(1,3299)	1:A:247:THR:HG21	1:A:263:GLU:HB3	11	0.11
(1,3299)	1:A:247:THR:HG21	1:B:277:LEU:HB3	11	0.11
(1,3068)	1:B:251:ILE:HD11	1:B:234:LEU:HB3	4	0.11
(1,3068)	1:B:251:ILE:HD11	1:B:251:ILE:HB	4	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG22	19	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG21	19	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HG23	19	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD12	19	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD11	19	0.11
(1,3014)	1:B:231:ASP:HA	1:B:251:ILE:HD13	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG22	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG21	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HG23	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD12	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD11	19	0.11
(1,3013)	1:A:231:ASP:HA	1:A:251:ILE:HD13	19	0.11
(1,2914)	1:B:282:SER:H	1:B:280:ARG:HB3	10	0.11
(1,2913)	1:A:282:SER:H	1:A:280:ARG:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2688)	1:B:281:GLU:H	1:B:281:GLU:HB2	15	0.11
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	3	0.11
(1,2648)	1:B:279:GLU:H	1:B:279:GLU:HB2	12	0.11
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	3	0.11
(1,2647)	1:A:279:GLU:H	1:A:279:GLU:HB2	6	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	1	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	2	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	8	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	10	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	13	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	15	0.11
(1,2542)	1:B:274:LEU:H	1:B:274:LEU:HB3	17	0.11
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	1	0.11
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	2	0.11
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	8	0.11
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	13	0.11
(1,2541)	1:A:274:LEU:H	1:A:274:LEU:HB3	17	0.11
(1,24)	1:B:264:PHE:HE1	1:B:270:LEU:HD11	18	0.11
(1,2354)	1:B:265:PHE:H	1:B:266:SER:H	15	0.11
(1,23)	1:A:264:PHE:HE1	1:A:270:LEU:HD11	18	0.11
(1,2278)	1:B:264:PHE:H	1:A:254:GLN:HB3	18	0.11
(1,2020)	1:B:254:GLN:HE21	1:B:257:LYS:HB3	1	0.11
(1,1826)	1:B:249:VAL:H	1:B:249:VAL:HG21	4	0.11
(1,1803)	1:A:248:THR:H	1:A:262:ILE:HG21	5	0.11
(1,1400)	1:B:234:LEU:H	1:B:234:LEU:HD21	17	0.11
(1,1399)	1:A:234:LEU:H	1:A:234:LEU:HD21	17	0.11
(1,1208)	1:B:274:LEU:HD21	1:A:237:ARG:HD2	11	0.11
(1,1207)	1:A:274:LEU:HD21	1:B:237:ARG:HD2	11	0.11
(1,1160)	1:B:251:ILE:HD11	1:A:264:PHE:HE2	9	0.11
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD22	12	0.11
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD21	12	0.11
(1,1114)	1:B:279:GLU:HB3	1:A:276:LEU:HD23	12	0.11
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD22	12	0.11
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD21	12	0.11
(1,1113)	1:A:279:GLU:HB3	1:B:276:LEU:HD23	12	0.11
(1,1044)	1:B:234:LEU:HB3	1:A:270:LEU:HD11	7	0.11
(1,1043)	1:A:234:LEU:HB3	1:B:270:LEU:HD11	19	0.11
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	6	0.11
(1,1036)	1:B:260:ILE:HG21	1:B:260:ILE:HB	11	0.11
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	6	0.11
(1,1035)	1:A:260:ILE:HG21	1:A:260:ILE:HB	11	0.11

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

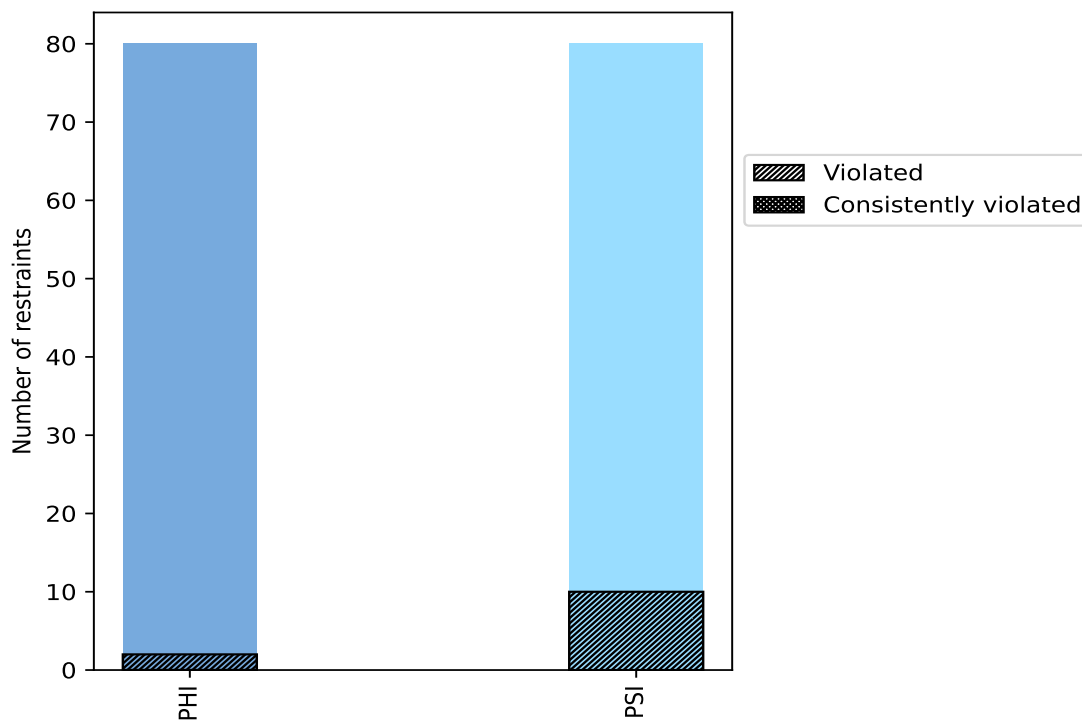
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	80	50.0	2	2.5	1.2	0	0.0	0.0
PSI	80	50.0	10	12.5	6.2	0	0.0	0.0
Total	160	100.0	12	7.5	7.5	0	0.0	0.0

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](#)



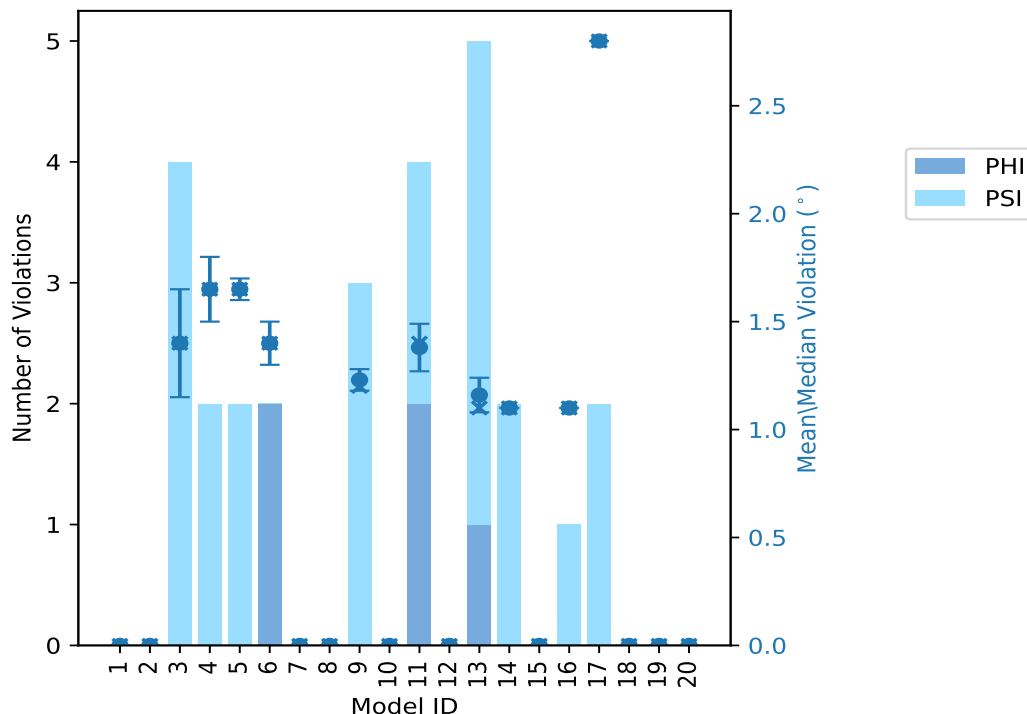
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	4	4	1.4	1.7	0.25	1.4
4	0	2	2	1.65	1.8	0.15	1.65
5	0	2	2	1.65	1.7	0.05	1.65
6	2	0	2	1.4	1.5	0.1	1.4
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	3	3	1.23	1.3	0.05	1.2
10	0	0	0	0.0	0.0	0.0	0.0
11	2	2	4	1.38	1.5	0.11	1.4
12	0	0	0	0.0	0.0	0.0	0.0
13	1	4	5	1.16	1.3	0.08	1.1
14	0	2	2	1.1	1.1	0.0	1.1
15	0	0	0	0.0	0.0	0.0	0.0
16	0	1	1	1.1	1.1	0.0	1.1
17	0	2	2	2.8	2.8	0.0	2.8
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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



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

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

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

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

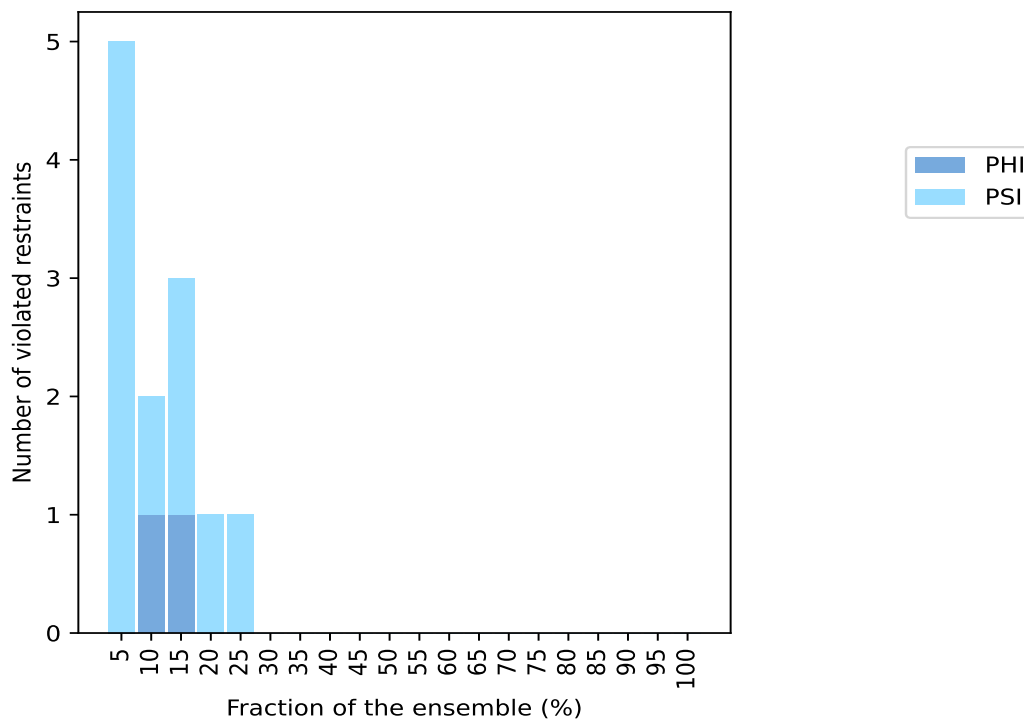
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

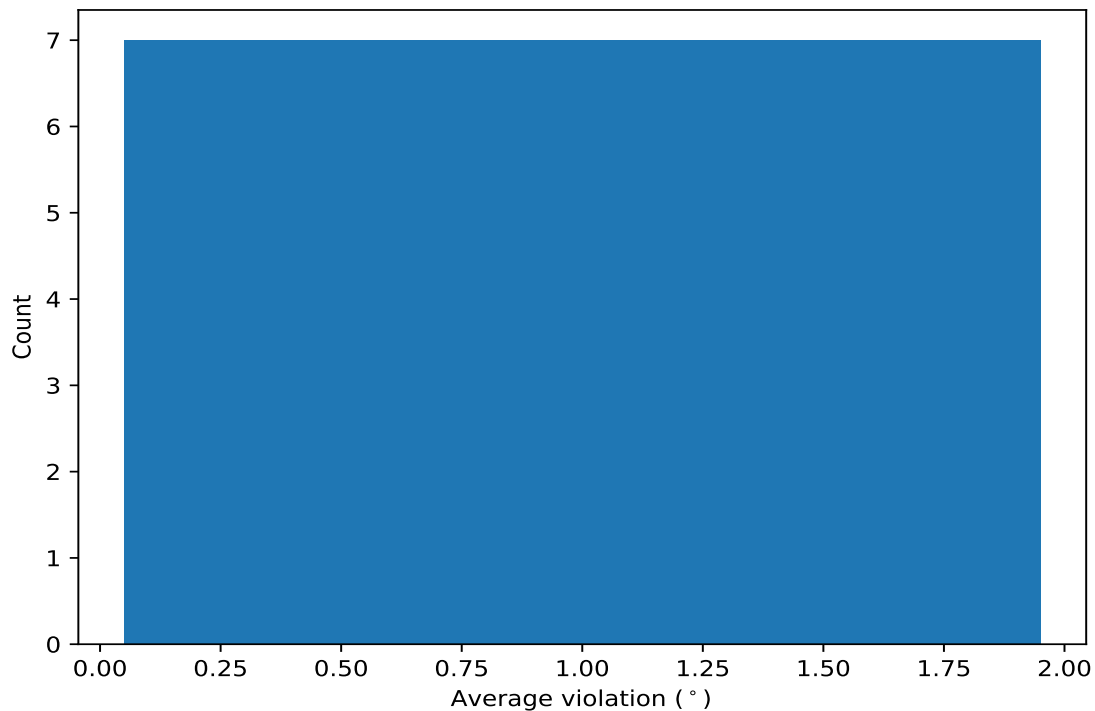


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

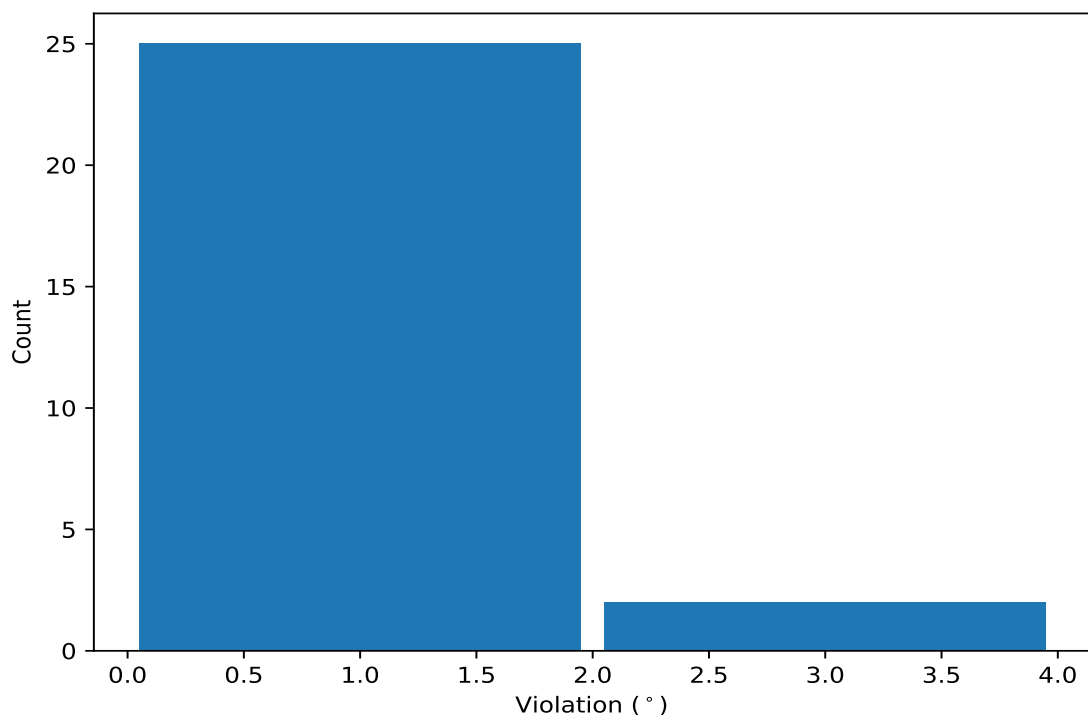
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	5	1.26	0.21	1.1
(1,58)	1:A:264:PHE:N	1:A:264:PHE:CA	1:A:264:PHE:C	1:A:265:PHE:N	4	1.3	0.23	1.2
(1,110)	1:B:245:PHE:N	1:B:245:PHE:CA	1:B:245:PHE:C	1:B:246:GLY:N	3	1.87	0.7	1.7
(1,30)	1:A:245:PHE:N	1:A:245:PHE:CA	1:A:245:PHE:C	1:A:246:GLY:N	3	1.83	0.71	1.6
(1,13)	1:A:236:GLU:C	1:A:237:ARG:N	1:A:237:ARG:CA	1:A:237:ARG:C	3	1.4	0.14	1.5
(1,114)	1:B:247:THR:N	1:B:247:THR:CA	1:B:247:THR:C	1:B:248:THR:N	2	1.55	0.25	1.55
(1,93)	1:B:236:GLU:C	1:B:237:ARG:N	1:B:237:ARG:CA	1:B:237:ARG:C	2	1.35	0.05	1.35

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 (°)
(1,30)	1:A:245:PHE:N	1:A:245:PHE:CA	1:A:245:PHE:C	1:A:246:GLY:N	17	2.8
(1,110)	1:B:245:PHE:N	1:B:245:PHE:CA	1:B:245:PHE:C	1:B:246:GLY:N	17	2.8
(1,114)	1:B:247:THR:N	1:B:247:THR:CA	1:B:247:THR:C	1:B:248:THR:N	4	1.8
(1,58)	1:A:264:PHE:N	1:A:264:PHE:CA	1:A:264:PHE:C	1:A:265:PHE:N	5	1.7
(1,110)	1:B:245:PHE:N	1:B:245:PHE:CA	1:B:245:PHE:C	1:B:246:GLY:N	3	1.7
(1,30)	1:A:245:PHE:N	1:A:245:PHE:CA	1:A:245:PHE:C	1:A:246:GLY:N	3	1.6
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	5	1.6
(1,34)	1:A:247:THR:N	1:A:247:THR:CA	1:A:247:THR:C	1:A:248:THR:N	4	1.5
(1,13)	1:A:236:GLU:C	1:A:237:ARG:N	1:A:237:ARG:CA	1:A:237:ARG:C	6	1.5
(1,13)	1:A:236:GLU:C	1:A:237:ARG:N	1:A:237:ARG:CA	1:A:237:ARG:C	11	1.5
(1,93)	1:B:236:GLU:C	1:B:237:ARG:N	1:B:237:ARG:CA	1:B:237:ARG:C	11	1.4
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	11	1.4
(1,93)	1:B:236:GLU:C	1:B:237:ARG:N	1:B:237:ARG:CA	1:B:237:ARG:C	6	1.3
(1,150)	1:B:272:ARG:N	1:B:272:ARG:CA	1:B:272:ARG:C	1:B:273:ILE:N	13	1.3
(1,114)	1:B:247:THR:N	1:B:247:THR:CA	1:B:247:THR:C	1:B:248:THR:N	9	1.3
(1,74)	1:A:274:LEU:N	1:A:274:LEU:CA	1:A:274:LEU:C	1:A:275:GLU:N	9	1.2
(1,58)	1:A:264:PHE:N	1:A:264:PHE:CA	1:A:264:PHE:C	1:A:265:PHE:N	3	1.2
(1,58)	1:A:264:PHE:N	1:A:264:PHE:CA	1:A:264:PHE:C	1:A:265:PHE:N	11	1.2
(1,154)	1:B:274:LEU:N	1:B:274:LEU:CA	1:B:274:LEU:C	1:B:275:GLU:N	9	1.2
(1,13)	1:A:236:GLU:C	1:A:237:ARG:N	1:A:237:ARG:CA	1:A:237:ARG:C	13	1.2
(1,70)	1:A:272:ARG:N	1:A:272:ARG:CA	1:A:272:ARG:C	1:A:273:ILE:N	13	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:A:264:PHE:N	1:A:264:PHE:CA	1:A:264:PHE:C	1:A:265:PHE:N	14	1.1
(1,30)	1:A:245:PHE:N	1:A:245:PHE:CA	1:A:245:PHE:C	1:A:246:GLY:N	13	1.1
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	3	1.1
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	14	1.1
(1,138)	1:B:264:PHE:N	1:B:264:PHE:CA	1:B:264:PHE:C	1:B:265:PHE:N	16	1.1
(1,110)	1:B:245:PHE:N	1:B:245:PHE:CA	1:B:245:PHE:C	1:B:246:GLY:N	13	1.1