



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:37 AM UTC

PDB ID : 2K7Z / pdb_00002k7z
BMRB ID : 15932
Title : Solution Structure of the Catalytic Domain of Procaspase-8
Authors : Keller, N.; Zerbe, O.; Mares, J.; Gruetter, M.G.
Deposited on : 2008-08-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

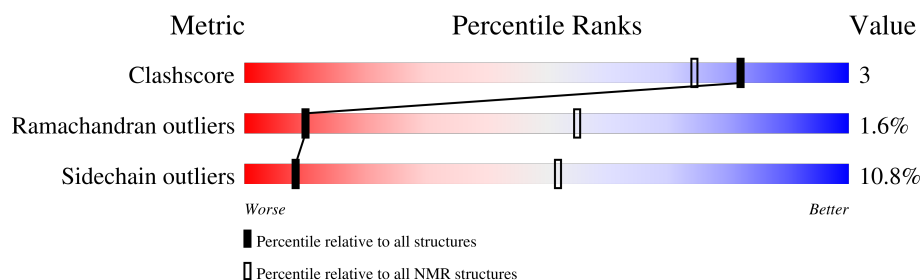
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	266	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:225-A:251, A:264-A:361, A:394-A:404, A:421-A:446, A:464-A:479 (178)	2.15	1

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3622 atoms, of which 1795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Caspase-8.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3622	1160	1795	305	349	13	

There are 4 discrepancies between the modelled and reference sequences:

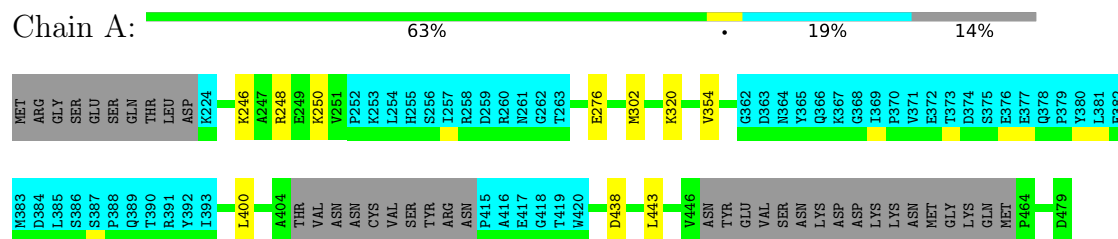
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	expression tag	UNP Q14790
A	215	ARG	-	expression tag	UNP Q14790
A	216	GLY	-	expression tag	UNP Q14790
A	360	ALA	CYS	engineered mutation	UNP Q14790

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: Caspase-8

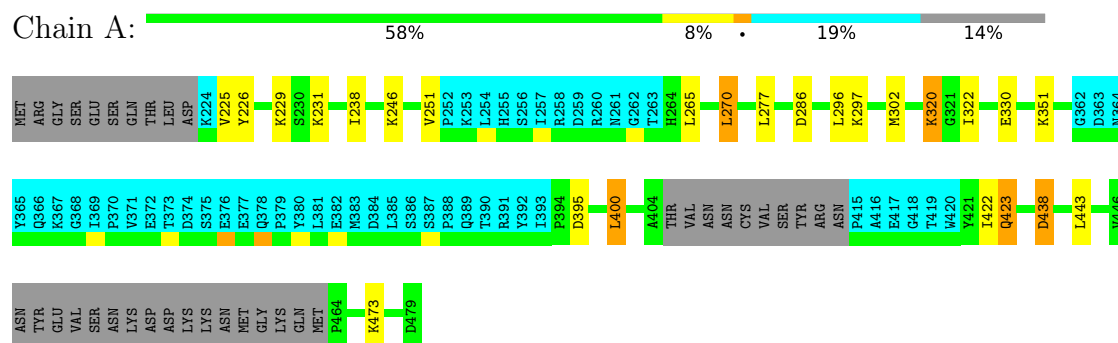


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

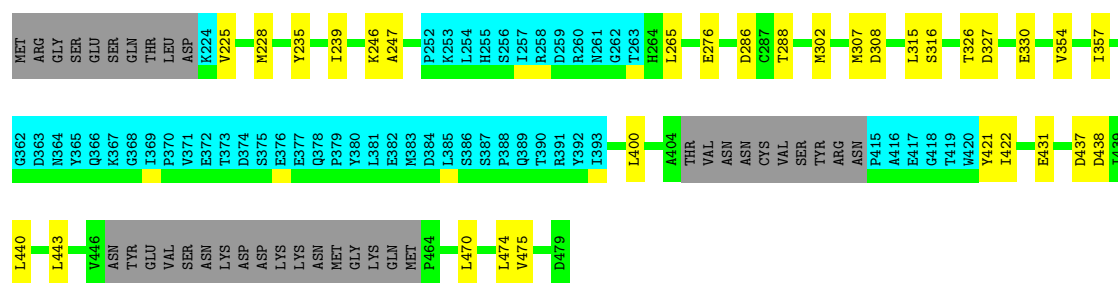
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Caspase-8



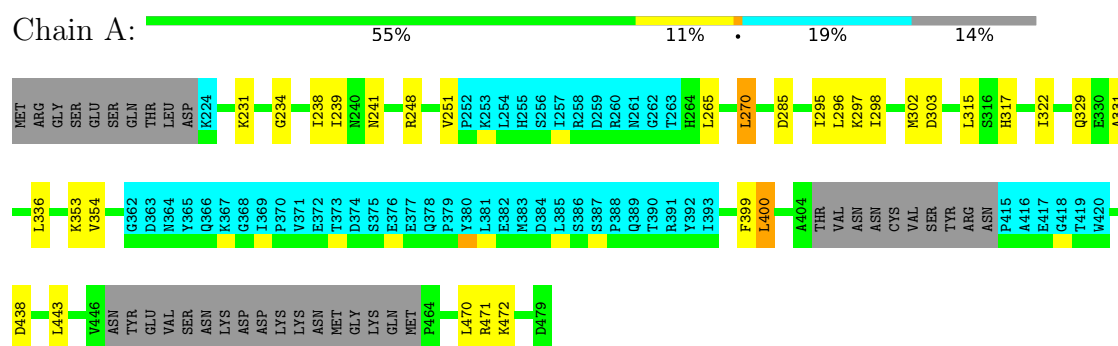
4.2.2 Score per residue for model 2

- Molecule 1: Caspase-8



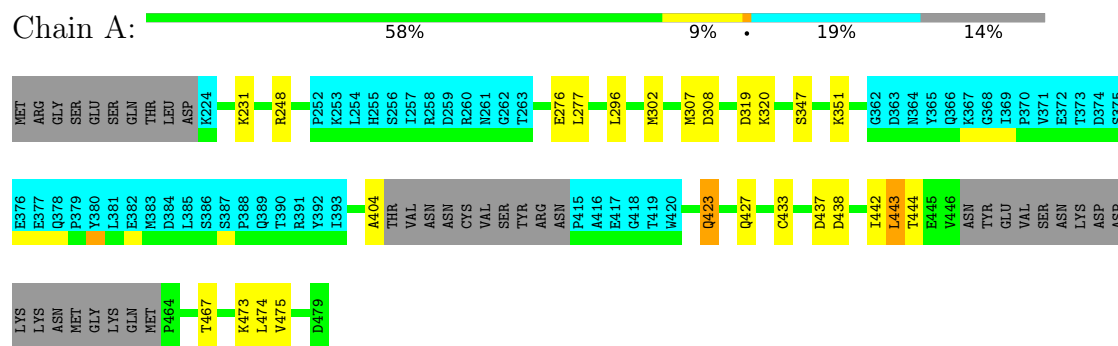
4.2.6 Score per residue for model 6

- Molecule 1: Caspase-8



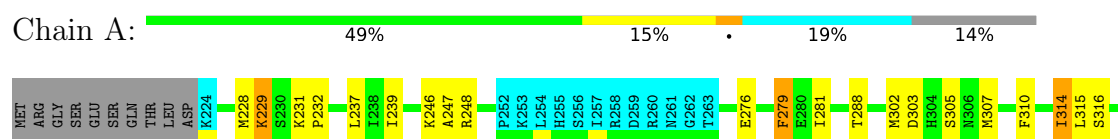
4.2.7 Score per residue for model 7

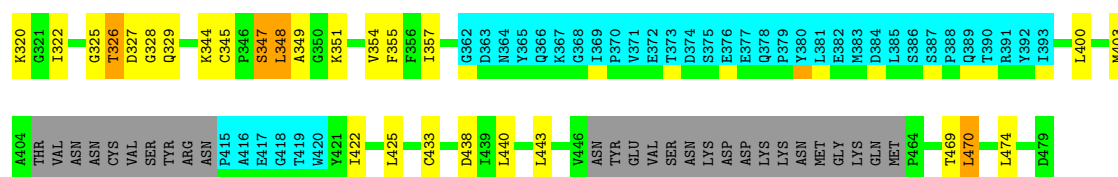
- Molecule 1: Caspase-8



4.2.8 Score per residue for model 8

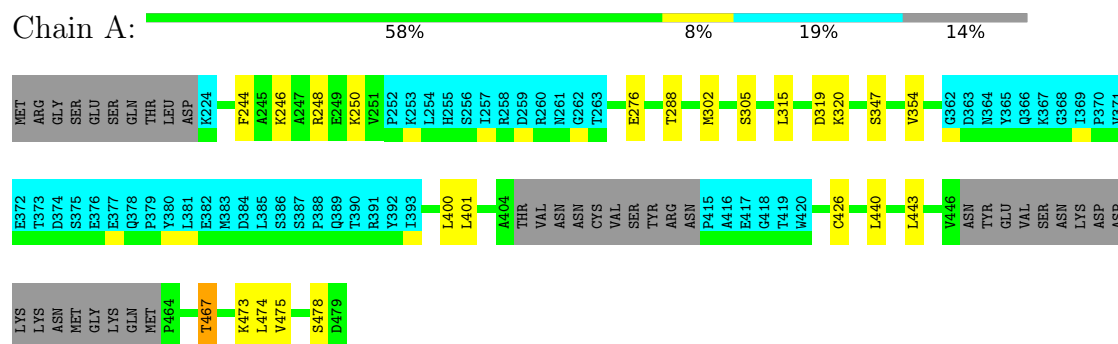
- Molecule 1: Caspase-8





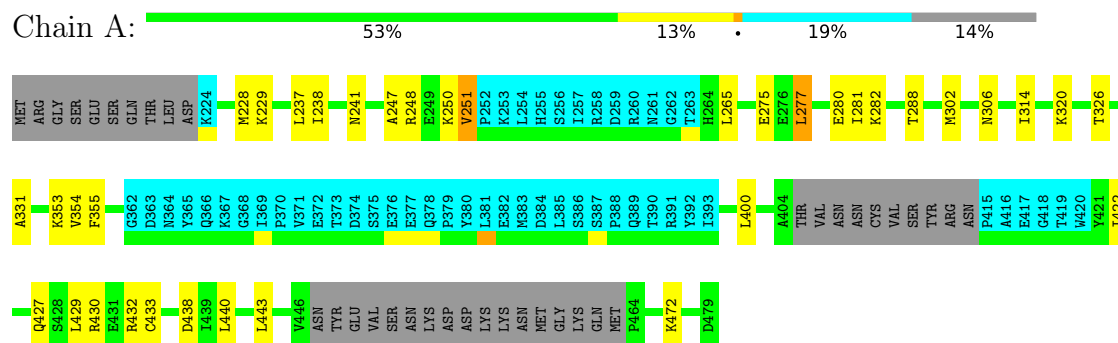
4.2.9 Score per residue for model 9

- Molecule 1: Caspase-8



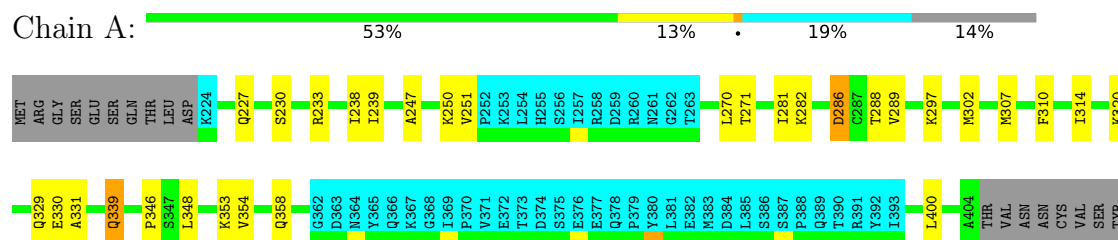
4.2.10 Score per residue for model 10

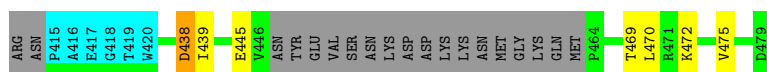
- Molecule 1: Caspase-8



4.2.11 Score per residue for model 11

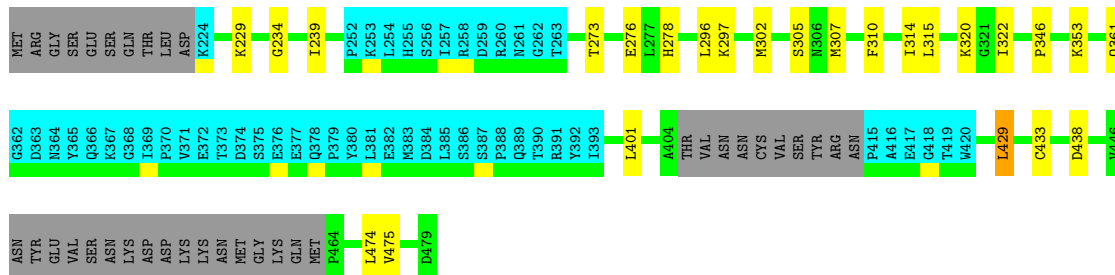
- Molecule 1: Caspase-8





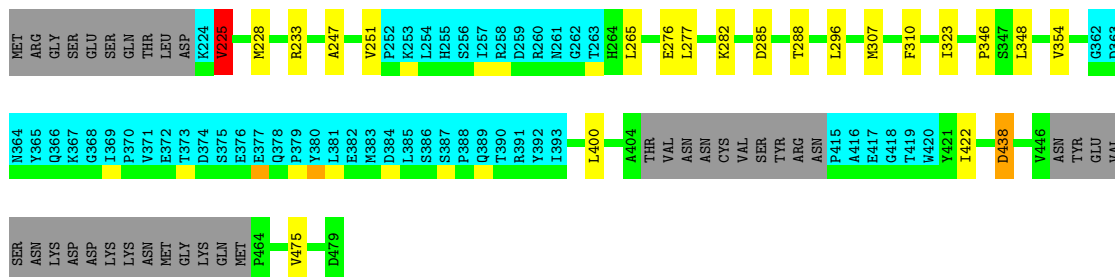
4.2.12 Score per residue for model 12

- Molecule 1: Caspase-8



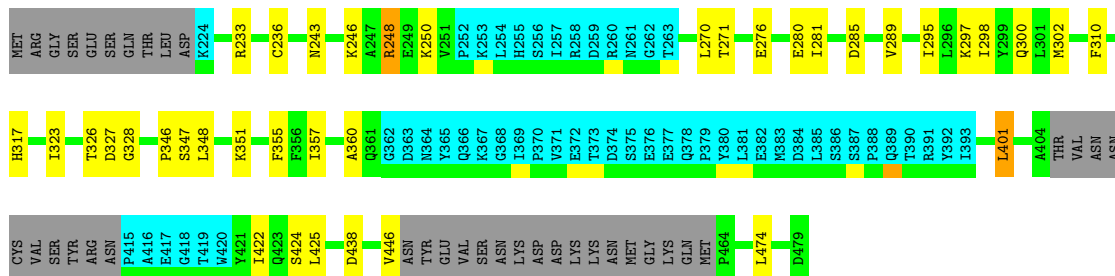
4.2.13 Score per residue for model 13

- Molecule 1: Caspase-8



4.2.14 Score per residue for model 14

- Molecule 1: Caspase-8



4.2.15 Score per residue for model 15

- Molecule 1: Caspase-8

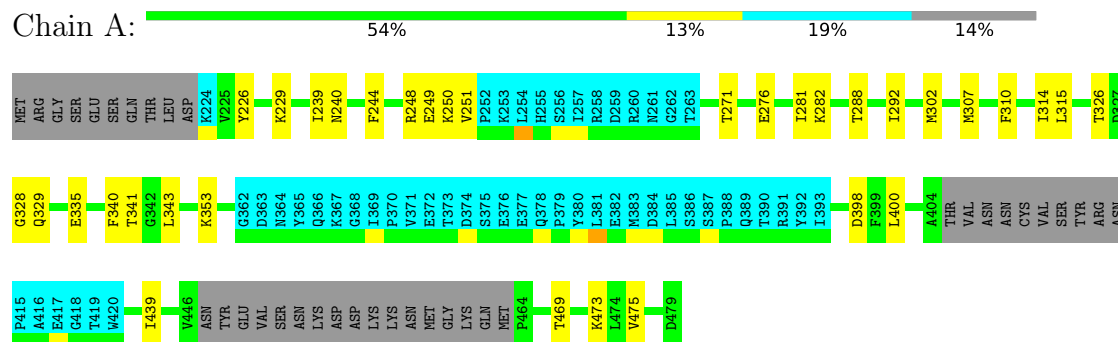
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Caspase-8

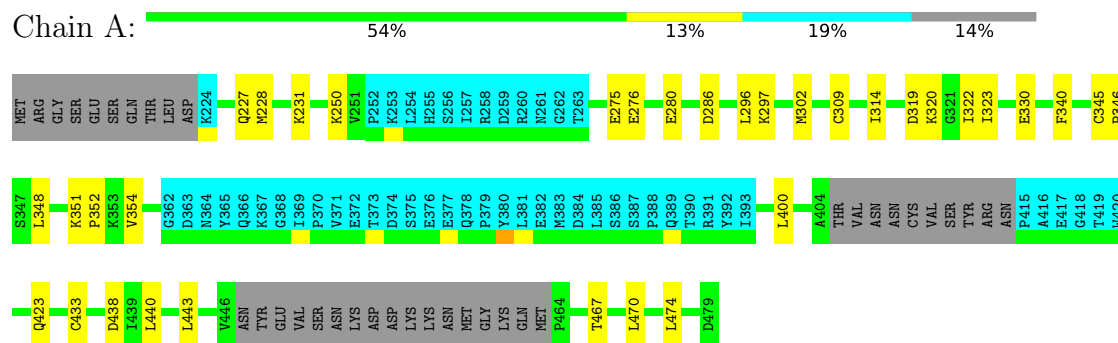
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Caspase-8

Chain A:



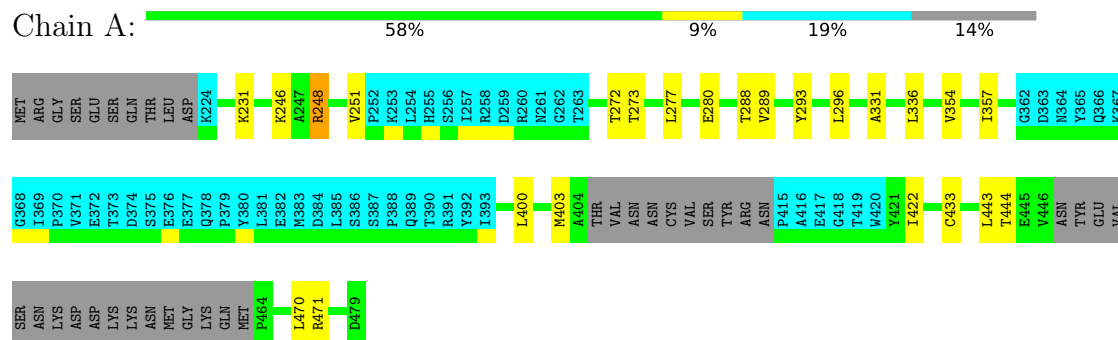
4.2.18 Score per residue for model 18

• Molecule 1: Caspase-8



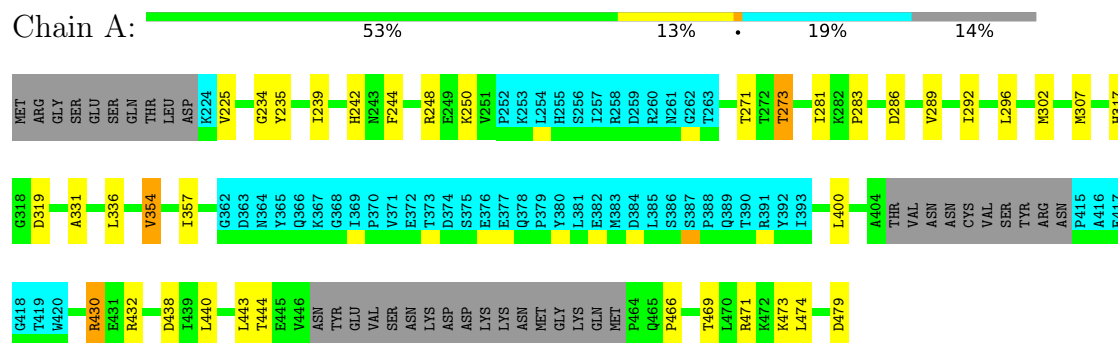
4.2.19 Score per residue for model 19

• Molecule 1: Caspase-8



4.2.20 Score per residue for model 20

• Molecule 1: Caspase-8



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	geometry optimization	6.0
CYANA	structure solution	2.2
CYANA	refinement	2.2

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	2477
Number of shifts mapped to atoms	2474
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.78±0.01	0±0/1446 (0.0± 0.0%)	1.26±0.02	1±1/1951 (0.1± 0.0%)
All	All	0.78	0/28920 (0.0%)	1.26	28/39020 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	286	ASP	CA-CB-CG	7.64	120.24	112.60	17	2
1	A	438	ASP	CA-CB-CG	7.49	120.09	112.60	17	7
1	A	398	ASP	CA-CB-CG	6.69	119.29	112.60	16	1
1	A	272	THR	CA-C-N	6.60	129.45	120.54	19	1
1	A	272	THR	C-N-CA	6.60	129.45	120.54	19	1
1	A	319	ASP	CA-CB-CG	-6.52	106.08	112.60	7	1
1	A	479	ASP	CA-CB-CG	6.28	118.88	112.60	20	2
1	A	303	ASP	CA-CB-CG	6.11	118.71	112.60	6	1
1	A	251	VAL	CA-C-N	5.47	126.67	119.84	10	1
1	A	251	VAL	C-N-CA	5.47	126.67	119.84	10	1
1	A	331	ALA	N-CA-C	5.46	113.14	108.22	6	3
1	A	346	PRO	CA-C-N	5.42	127.85	120.54	12	2
1	A	346	PRO	C-N-CA	5.42	127.85	120.54	12	2
1	A	395	ASP	CA-CB-CG	5.13	117.73	112.60	1	1
1	A	344	LYS	CA-C-N	5.00	126.68	122.28	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	344	LYS	C-N-CA	5.00	126.68	122.28	8	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	421	TYR	Sidechain	1

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	1416	1407	1407	7±4
All	All	28320	28140	28140	142

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:LEU:HD11	1:A:443:LEU:HD11	0.91	1.42	9	4
1:A:354:VAL:HG23	1:A:400:LEU:HD12	0.79	1.55	20	1
1:A:354:VAL:HG13	1:A:400:LEU:HD12	0.77	1.53	9	5
1:A:225:VAL:HG22	1:A:228:MET:HE2	0.67	1.65	5	1
1:A:277:LEU:HD11	1:A:433:CYS:HB3	0.67	1.65	19	1
1:A:271:THR:HG23	1:A:281:ILE:HG21	0.66	1.67	16	6
1:A:400:LEU:HD11	1:A:443:LEU:CD1	0.64	2.23	20	1
1:A:440:LEU:HD11	1:A:470:LEU:HD13	0.62	1.70	5	1
1:A:238:ILE:HD12	1:A:270:LEU:HD13	0.61	1.70	6	1
1:A:225:VAL:HG21	1:A:475:VAL:HG23	0.60	1.71	13	1
1:A:440:LEU:HD13	1:A:470:LEU:HD12	0.59	1.74	18	1
1:A:438:ASP:HA	1:A:475:VAL:HG22	0.58	1.75	5	1
1:A:234:GLY:HA2	1:A:307:MET:HE1	0.58	1.74	4	1
1:A:404:ALA:HB3	1:A:467:THR:HG22	0.56	1.76	7	1
1:A:438:ASP:HB3	1:A:475:VAL:HG22	0.56	1.78	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:THR:HG22	1:A:466:PRO:HB2	0.56	1.77	20	1
1:A:235:TYR:CD2	1:A:307:MET:HE2	0.55	2.37	5	1
1:A:331:ALA:HB1	1:A:336:LEU:HD11	0.54	1.80	20	1
1:A:239:ILE:HG21	1:A:292:ILE:HD11	0.54	1.77	16	2
1:A:340:PHE:O	1:A:349:ALA:HB2	0.53	2.03	2	1
1:A:400:LEU:HD23	1:A:440:LEU:HD23	0.53	1.78	8	1
1:A:289:VAL:HG11	1:A:329:GLN:HB2	0.53	1.78	11	1
1:A:440:LEU:HD11	1:A:470:LEU:CD1	0.53	2.34	5	1
1:A:331:ALA:HB3	1:A:336:LEU:HD11	0.53	1.78	19	1
1:A:233:ARG:O	1:A:307:MET:HE1	0.53	2.04	11	1
1:A:444:THR:HG22	1:A:466:PRO:CB	0.52	2.35	20	1
1:A:354:VAL:CG2	1:A:474:LEU:HD21	0.52	2.35	17	1
1:A:400:LEU:HD21	1:A:443:LEU:HD11	0.51	1.82	10	1
1:A:239:ILE:HD13	1:A:314:ILE:CD1	0.51	2.36	12	2
1:A:438:ASP:CB	1:A:475:VAL:HG22	0.51	2.35	13	3
1:A:289:VAL:CG2	1:A:331:ALA:HB2	0.51	2.36	11	1
1:A:225:VAL:HG23	1:A:475:VAL:HG21	0.49	1.84	18	1
1:A:352:PRO:HB3	1:A:470:LEU:HD23	0.49	1.84	2	2
1:A:281:ILE:HD12	1:A:281:ILE:H	0.49	1.67	18	1
1:A:440:LEU:HD21	1:A:470:LEU:HD13	0.48	1.84	2	1
1:A:323:ILE:HD12	1:A:323:ILE:H	0.48	1.68	17	1
1:A:355:PHE:HB2	1:A:401:LEU:HD12	0.47	1.86	14	1
1:A:238:ILE:C	1:A:239:ILE:HD12	0.47	2.34	11	2
1:A:239:ILE:HD13	1:A:314:ILE:HD13	0.47	1.87	12	1
1:A:247:ALA:HB1	1:A:251:VAL:HG23	0.47	1.87	10	1
1:A:279:PHE:CE1	1:A:281:ILE:HD11	0.47	2.44	2	2
1:A:273:THR:HG21	1:A:429:LEU:HD11	0.47	1.87	12	1
1:A:239:ILE:HG22	1:A:315:LEU:HD13	0.46	1.85	5	1
1:A:225:VAL:HG23	1:A:473:LYS:HG2	0.46	1.87	2	1
1:A:354:VAL:HG13	1:A:400:LEU:HD23	0.46	1.88	10	1
1:A:360:ALA:CB	1:A:422:ILE:HG21	0.46	2.40	4	1
1:A:303:ASP:HA	1:A:348:LEU:HD21	0.45	1.86	8	1
1:A:236:CYS:SG	1:A:281:ILE:HG23	0.45	2.51	14	1
1:A:288:THR:HA	1:A:326:THR:HG21	0.45	1.88	8	1
1:A:357:ILE:HD13	1:A:403:MET:HE2	0.45	1.87	8	1
1:A:273:THR:HG21	1:A:430:ARG:HB2	0.45	1.87	20	1
1:A:345:CYS:O	1:A:349:ALA:HB2	0.45	2.12	8	2
1:A:326:THR:HG22	1:A:328:GLY:H	0.45	1.71	14	1
1:A:422:ILE:HG22	1:A:425:LEU:HD13	0.45	1.88	14	1
1:A:234:GLY:HA2	1:A:307:MET:HE3	0.45	1.89	20	1
1:A:400:LEU:HD13	1:A:440:LEU:HD23	0.45	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:TYR:CD2	1:A:307:MET:HE1	0.45	2.46	20	1
1:A:422:ILE:HD12	1:A:422:ILE:H	0.44	1.72	19	2
1:A:400:LEU:CD1	1:A:443:LEU:HD11	0.44	2.41	2	1
1:A:354:VAL:HG13	1:A:400:LEU:HD11	0.44	1.87	6	1
1:A:401:LEU:HD22	1:A:467:THR:HB	0.44	1.89	9	1
1:A:238:ILE:HD13	1:A:270:LEU:HB2	0.44	1.89	1	1
1:A:348:LEU:HD23	1:A:351:LYS:CE	0.44	2.42	14	1
1:A:240:ASN:CG	1:A:267:ALA:HB2	0.44	2.38	18	1
1:A:289:VAL:HG12	1:A:293:TYR:CE1	0.44	2.48	19	1
1:A:247:ALA:HB2	1:A:327:ASP:OD2	0.44	2.13	5	1
1:A:225:VAL:HG22	1:A:226:TYR:CD2	0.44	2.48	1	1
1:A:239:ILE:HG21	1:A:292:ILE:CD1	0.44	2.43	16	1
1:A:237:LEU:HD13	1:A:282:LYS:HB3	0.43	1.91	10	1
1:A:277:LEU:HD21	1:A:433:CYS:HB3	0.43	1.90	10	1
1:A:251:VAL:CG2	1:A:322:ILE:HD13	0.43	2.43	2	1
1:A:238:ILE:HD12	1:A:281:ILE:HG21	0.43	1.90	3	2
1:A:348:LEU:HD23	1:A:351:LYS:HE2	0.43	1.91	14	1
1:A:438:ASP:OD1	1:A:473:LYS:HE3	0.43	2.14	7	1
1:A:360:ALA:HB2	1:A:422:ILE:HD11	0.43	1.90	14	1
1:A:400:LEU:HD13	1:A:400:LEU:C	0.42	2.39	5	1
1:A:347:SER:C	1:A:348:LEU:HD22	0.42	2.39	8	1
1:A:352:PRO:CB	1:A:470:LEU:HD23	0.42	2.44	2	1
1:A:394:PRO:HD2	1:A:401:LEU:HD22	0.42	1.91	3	1
1:A:316:SER:OG	1:A:330:GLU:OE1	0.42	2.37	5	1
1:A:422:ILE:HD12	1:A:425:LEU:HD23	0.42	1.91	8	1
1:A:425:LEU:HD13	1:A:446:VAL:HG11	0.42	1.91	15	1
1:A:225:VAL:HG21	1:A:473:LYS:HG2	0.42	1.89	20	1
1:A:438:ASP:OD2	1:A:473:LYS:HE3	0.42	2.15	1	1
1:A:400:LEU:HD23	1:A:440:LEU:HD22	0.42	1.90	20	1
1:A:295:ILE:HA	1:A:298:ILE:HD12	0.42	1.92	14	3
1:A:247:ALA:HB1	1:A:251:VAL:CG2	0.42	2.45	11	2
1:A:281:ILE:HG22	1:A:283:PRO:HD3	0.42	1.90	20	1
1:A:239:ILE:HD13	1:A:314:ILE:HG23	0.42	1.92	8	1
1:A:473:LYS:HG2	1:A:475:VAL:HG23	0.42	1.91	9	1
1:A:244:PHE:HA	1:A:247:ALA:HB3	0.42	1.91	15	1
1:A:400:LEU:HB2	1:A:470:LEU:HD11	0.42	1.92	18	1
1:A:237:LEU:HD23	1:A:310:PHE:CZ	0.42	2.50	8	1
1:A:440:LEU:HD23	1:A:470:LEU:HD13	0.41	1.91	17	1
1:A:400:LEU:HD21	1:A:443:LEU:CD1	0.41	2.45	5	2
1:A:341:THR:HG22	1:A:343:LEU:H	0.41	1.75	16	1
1:A:225:VAL:HG11	1:A:475:VAL:HB	0.41	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:293:TYR:CE1	1:A:336:LEU:HD21	0.41	2.50	15	1
1:A:245:ALA:O	1:A:246:LYS:HE2	0.41	2.16	18	1
1:A:424:SER:HB2	1:A:446:VAL:HG13	0.41	1.93	14	1
1:A:473:LYS:HE3	1:A:475:VAL:CG2	0.41	2.44	16	1
1:A:273:THR:HG23	1:A:430:ARG:HB3	0.41	1.92	2	1
1:A:226:TYR:HE1	1:A:475:VAL:HG21	0.41	1.76	15	1
1:A:273:THR:HG23	1:A:430:ARG:CB	0.41	2.46	18	1
1:A:319:ASP:OD1	1:A:320:LYS:HE3	0.41	2.16	3	1
1:A:314:ILE:HD13	1:A:355:PHE:CE1	0.41	2.51	10	1
1:A:354:VAL:HG13	1:A:400:LEU:CD2	0.40	2.46	10	1
1:A:355:PHE:CE2	1:A:403:MET:HE3	0.40	2.51	8	1
1:A:307:MET:HE3	1:A:310:PHE:CZ	0.40	2.51	12	1
1:A:440:LEU:HD21	1:A:470:LEU:CD1	0.40	2.46	8	1
1:A:440:LEU:HD21	1:A:474:LEU:HB3	0.40	1.92	9	1
1:A:357:ILE:HG21	1:A:403:MET:CG	0.40	2.46	19	1
1:A:317:HIS:HB2	1:A:357:ILE:HD11	0.40	1.93	14	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	174/266 (65%)	151±4 (87±2%)	21±4 (12±2%)	3±2 (2±1%)	10	55
All	All	3480/5320 (65%)	3012 (87%)	411 (12%)	57 (2%)	10	55

All 35 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	234	GLY	4
1	A	328	GLY	4
1	A	347	SER	4
1	A	286	ASP	3
1	A	232	PRO	3
1	A	346	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	229	LYS	2
1	A	423	GLN	2
1	A	248	ARG	2
1	A	443	LEU	2
1	A	285	ASP	2
1	A	325	GLY	2
1	A	422	ILE	2
1	A	320	LYS	1
1	A	226	TYR	1
1	A	465	GLN	1
1	A	324	TYR	1
1	A	241	ASN	1
1	A	336	LEU	1
1	A	442	ILE	1
1	A	444	THR	1
1	A	306	ASN	1
1	A	432	ARG	1
1	A	339	GLN	1
1	A	225	VAL	1
1	A	233	ARG	1
1	A	323	ILE	1
1	A	264	HIS	1
1	A	321	GLY	1
1	A	345	CYS	1
1	A	227	GLN	1
1	A	228	MET	1
1	A	280	GLU	1
1	A	309	CYS	1
1	A	331	ALA	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/239 (66%)	141±4 (89±2%)	17±4 (11±2%)	8	52
All	All	3160/4780 (66%)	2818 (89%)	342 (11%)	8	52

All 99 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	302	MET	17
1	A	276	GLU	14
1	A	320	LYS	11
1	A	250	LYS	11
1	A	246	LYS	10
1	A	296	LEU	9
1	A	231	LYS	8
1	A	297	LYS	8
1	A	353	LYS	8
1	A	474	LEU	8
1	A	288	THR	8
1	A	248	ARG	8
1	A	400	LEU	7
1	A	443	LEU	7
1	A	351	LYS	6
1	A	280	GLU	6
1	A	433	CYS	6
1	A	322	ILE	5
1	A	314	ILE	5
1	A	329	GLN	5
1	A	229	LYS	5
1	A	265	LEU	5
1	A	315	LEU	5
1	A	348	LEU	5
1	A	251	VAL	4
1	A	270	LEU	4
1	A	277	LEU	4
1	A	330	GLU	4
1	A	317	HIS	4
1	A	438	ASP	4
1	A	319	ASP	4
1	A	439	ILE	4
1	A	326	THR	4
1	A	470	LEU	4
1	A	471	ARG	4
1	A	307	MET	4
1	A	469	THR	4
1	A	282	LYS	4
1	A	310	PHE	4
1	A	423	GLN	3
1	A	227	GLN	3
1	A	272	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	429	LEU	3
1	A	357	ILE	3
1	A	472	LYS	3
1	A	228	MET	3
1	A	305	SER	3
1	A	275	GLU	3
1	A	401	LEU	3
1	A	340	PHE	3
1	A	339	GLN	2
1	A	432	ARG	2
1	A	308	ASP	2
1	A	437	ASP	2
1	A	347	SER	2
1	A	427	GLN	2
1	A	327	ASP	2
1	A	467	THR	2
1	A	478	SER	2
1	A	430	ARG	2
1	A	354	VAL	2
1	A	289	VAL	2
1	A	273	THR	2
1	A	422	ILE	1
1	A	395	ASP	1
1	A	425	LEU	1
1	A	236	CYS	1
1	A	398	ASP	1
1	A	338	SER	1
1	A	431	GLU	1
1	A	399	PHE	1
1	A	279	PHE	1
1	A	316	SER	1
1	A	244	PHE	1
1	A	426	CYS	1
1	A	241	ASN	1
1	A	230	SER	1
1	A	358	GLN	1
1	A	445	GLU	1
1	A	278	HIS	1
1	A	361	GLN	1
1	A	225	VAL	1
1	A	285	ASP	1
1	A	233	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	243	ASN	1
1	A	300	GLN	1
1	A	323	ILE	1
1	A	309	CYS	1
1	A	344	LYS	1
1	A	479	ASP	1
1	A	226	TYR	1
1	A	240	ASN	1
1	A	335	GLU	1
1	A	345	CYS	1
1	A	249	GLU	1
1	A	266	ASP	1
1	A	444	THR	1
1	A	242	HIS	1
1	A	286	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2477
Number of shifts mapped to atoms	2474
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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

- No matching atom found in the structure. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	447	ASN	HD21	7.477	0.020	2
1	A	447	ASN	HD22	6.829	0.020	2
1	A	447	ASN	ND2	111.888	0.400	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	218	-0.13 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	203	0.31 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	208	0.57 ± 0.15	Should be applied
^{15}N	201	0.89 ± 0.23	Should be applied

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 82%, i.e. 2000 atoms were assigned a chemical shift out of a possible 2444. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	859/880 (98%)	342/356 (96%)	351/356 (99%)	166/168 (99%)
Sidechain	1087/1359 (80%)	711/885 (80%)	373/430 (87%)	3/44 (7%)
Aromatic	54/205 (26%)	27/102 (26%)	27/97 (28%)	0/6 (0%)
Overall	2000/2444 (82%)	1080/1343 (80%)	751/883 (85%)	169/218 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 2474 atoms were assigned a chemical shift out of a possible 3125. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1043/1129 (92%)	416/457 (91%)	426/458 (93%)	201/214 (94%)
Sidechain	1355/1745 (78%)	890/1131 (79%)	459/553 (83%)	6/61 (10%)
Aromatic	76/251 (30%)	38/124 (31%)	37/119 (31%)	1/8 (12%)
Overall	2474/3125 (79%)	1344/1712 (79%)	922/1130 (82%)	208/283 (73%)

7.1.4 Statistically unusual chemical shifts [i](#)

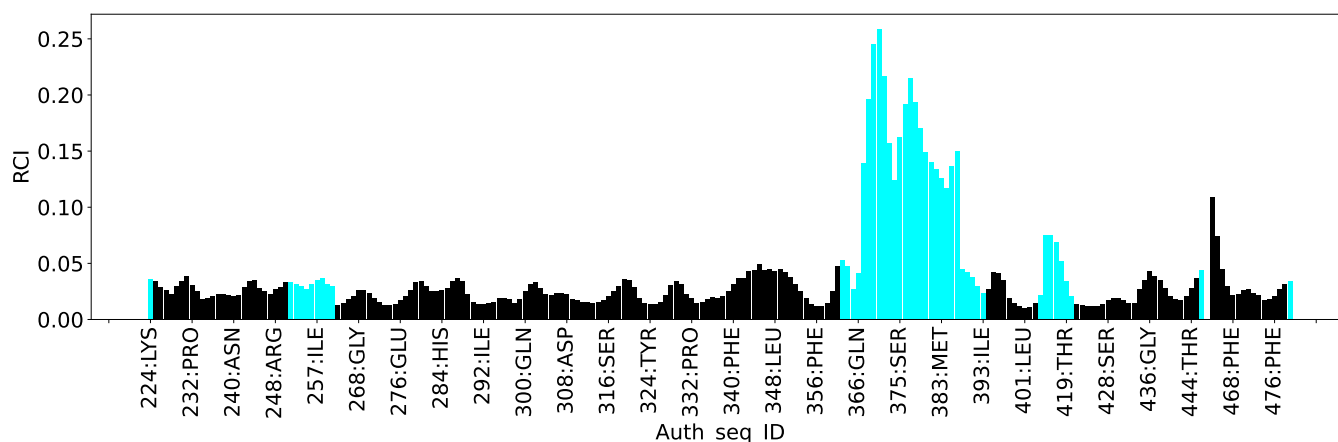
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	246	LYS	CE	58.01	37.57 – 46.21	18.7
1	A	422	ILE	CD1	29.95	5.18 – 21.60	10.1
1	A	472	LYS	HB2	-0.12	0.58 – 2.97	-7.9
1	A	248	ARG	NH1	111.52	49.05 – 99.42	7.4
1	A	260	ARG	NH1	111.52	49.05 – 99.42	7.4
1	A	260	ARG	HD2	1.64	1.97 – 4.26	-6.5
1	A	234	GLY	N	128.53	91.59 – 127.52	5.3
1	A	311	ILE	HD11	-0.73	-0.72 – 2.09	-5.0
1	A	311	ILE	HD12	-0.73	-0.72 – 2.09	-5.0
1	A	311	ILE	HD13	-0.73	-0.72 – 2.09	-5.0

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	2023
Intra-residue ($ i-j =0$)	532
Sequential ($ i-j =1$)	672
Medium range ($ i-j >1$ and $ i-j <5$)	405
Long range ($ i-j \geq 5$)	414
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	1
Number of restraints per residue	7.6
Number of long range restraints per residue ¹	1.6

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)	52.0	0.2
0.2-0.5 (Medium)	41.2	0.5
>0.5 (Large)	14.9	3.99

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

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

9 Distance violation analysis ⓘ

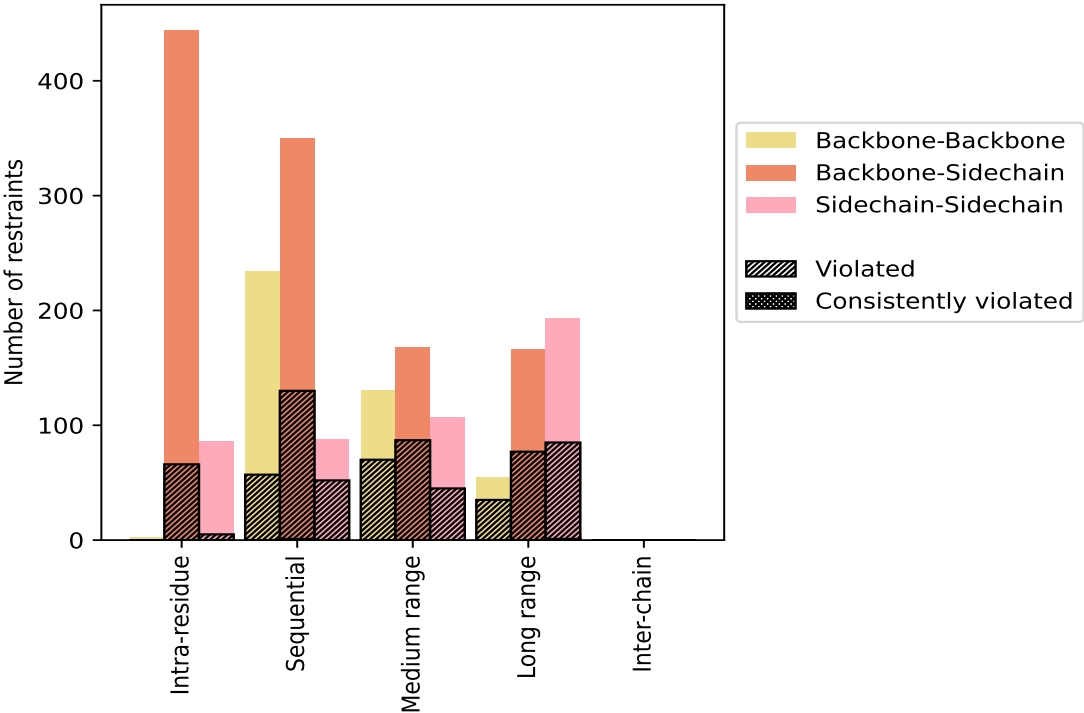
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	532	26.3	71	13.3	3.5	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	444	21.9	66	14.9	3.3	0	0.0	0.0
Sidechain-Sidechain	86	4.3	5	5.8	0.2	0	0.0	0.0
Sequential ($i-j =1$)	672	33.2	239	35.6	11.8	1	0.1	0.0
Backbone-Backbone	234	11.6	57	24.4	2.8	0	0.0	0.0
Backbone-Sidechain	350	17.3	130	37.1	6.4	1	0.3	0.0
Sidechain-Sidechain	88	4.3	52	59.1	2.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	405	20.0	202	49.9	10.0	0	0.0	0.0
Backbone-Backbone	130	6.4	70	53.8	3.5	0	0.0	0.0
Backbone-Sidechain	168	8.3	87	51.8	4.3	0	0.0	0.0
Sidechain-Sidechain	107	5.3	45	42.1	2.2	0	0.0	0.0
Long range ($i-j \geq 5$)	414	20.5	197	47.6	9.7	1	0.2	0.0
Backbone-Backbone	55	2.7	35	63.6	1.7	0	0.0	0.0
Backbone-Sidechain	166	8.2	77	46.4	3.8	0	0.0	0.0
Sidechain-Sidechain	193	9.5	85	44.0	4.2	1	0.5	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2023	100.0	709	35.0	35.0	2	0.1	0.1
Backbone-Backbone	421	20.8	162	38.5	8.0	0	0.0	0.0
Backbone-Sidechain	1128	55.8	360	31.9	17.8	1	0.1	0.0
Sidechain-Sidechain	474	23.4	187	39.5	9.2	1	0.2	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	9	31	23	17	0	80	0.46	3.29	0.69	0.21
2	10	26	36	30	0	102	0.46	2.91	0.68	0.24
3	8	46	29	27	0	110	0.33	3.32	0.44	0.2
4	15	36	36	30	0	117	0.38	3.83	0.54	0.2
5	11	39	36	25	0	111	0.32	2.56	0.36	0.21
6	15	37	44	39	0	135	0.41	3.99	0.64	0.19
7	11	38	39	26	0	114	0.39	3.93	0.65	0.2
8	11	30	29	33	0	103	0.41	3.16	0.56	0.23
9	10	26	36	24	0	96	0.35	2.88	0.47	0.2
10	5	38	32	20	0	95	0.22	0.65	0.12	0.18

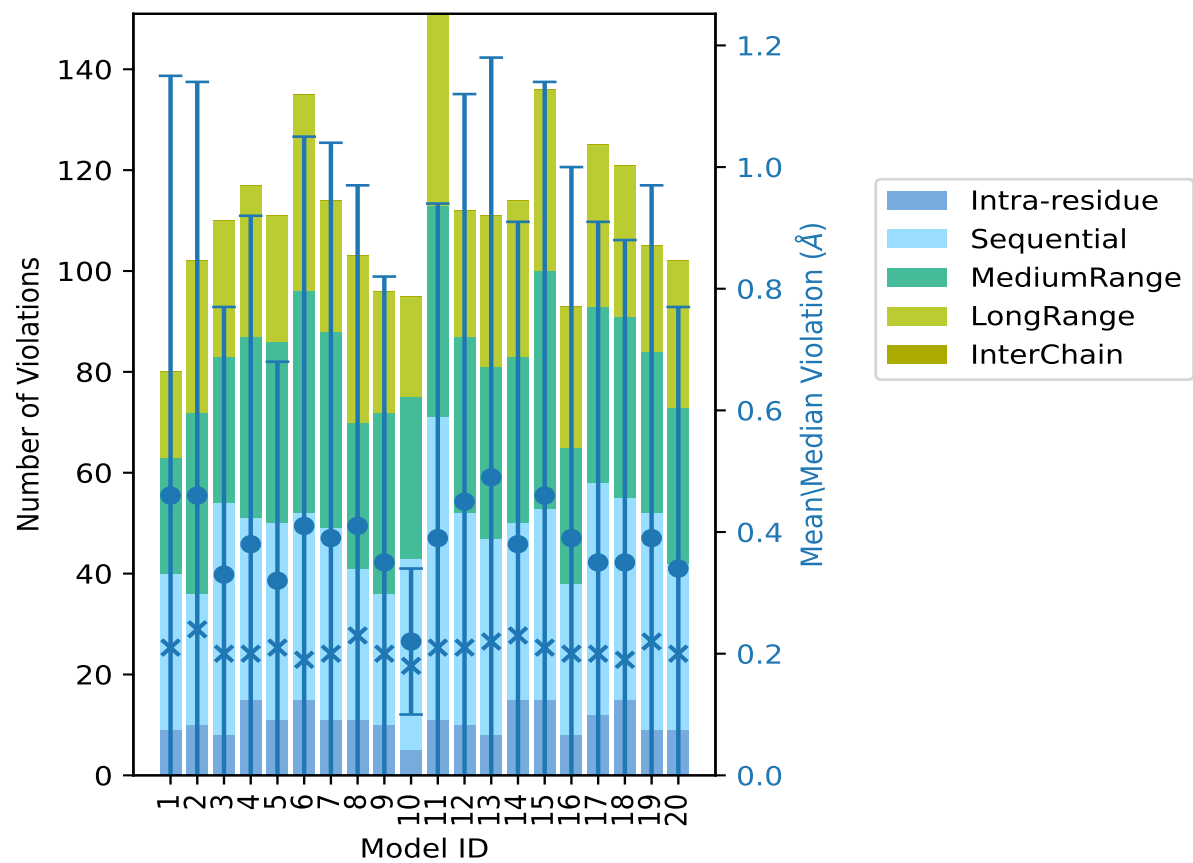
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	11	60	42	38	0	151	0.39	3.26	0.55	0.21
12	10	42	35	25	0	112	0.45	3.36	0.67	0.21
13	8	39	34	30	0	111	0.49	3.37	0.69	0.22
14	15	35	33	31	0	114	0.38	3.02	0.53	0.23
15	15	38	47	36	0	136	0.46	3.84	0.68	0.21
16	8	30	27	28	0	93	0.39	3.55	0.61	0.2
17	12	46	35	32	0	125	0.35	3.52	0.56	0.2
18	15	40	36	30	0	121	0.35	3.37	0.53	0.19
19	9	43	32	21	0	105	0.39	3.47	0.58	0.22
20	9	33	31	29	0	102	0.34	2.65	0.43	0.2

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

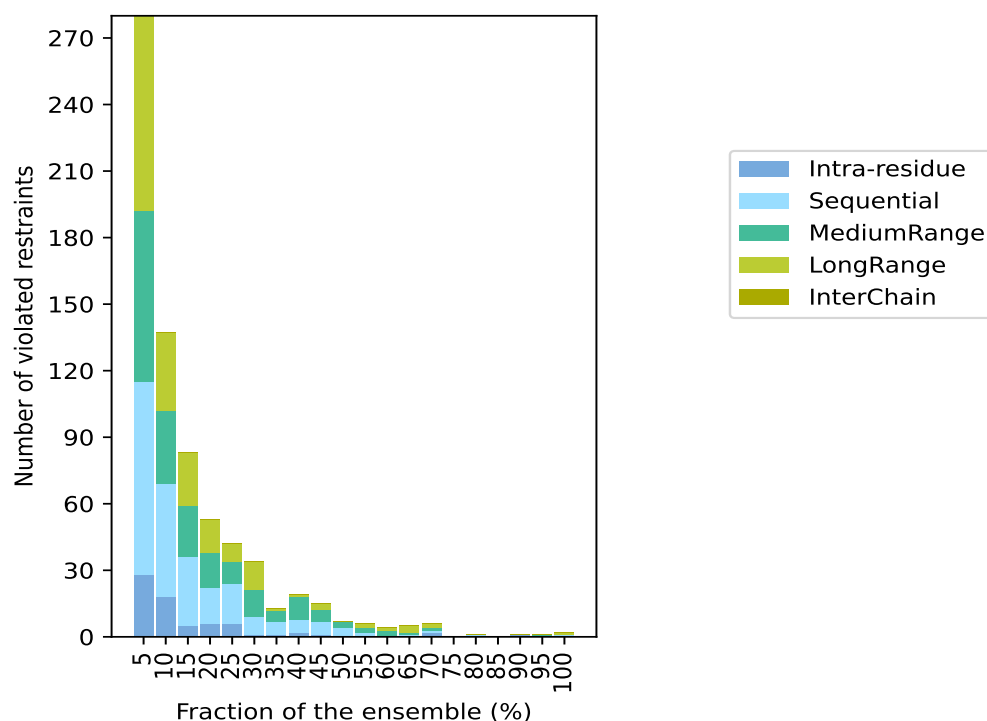
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1314(IR:461, SQ:433, MR:203, LR:217, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
28	87	77	88	0	280	1	5.0
18	51	33	35	0	137	2	10.0
5	31	23	24	0	83	3	15.0
6	16	16	15	0	53	4	20.0
6	18	10	8	0	42	5	25.0
1	8	12	13	0	34	6	30.0
1	6	5	1	0	13	7	35.0
2	6	10	1	0	19	8	40.0
1	6	5	3	0	15	9	45.0
0	4	3	0	0	7	10	50.0
0	2	2	2	0	6	11	55.0
0	0	3	1	0	4	12	60.0
0	1	1	3	0	5	13	65.0
2	1	1	2	0	6	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
1	0	0	0	0	1	18	90.0
0	0	1	0	0	1	19	95.0
0	1	0	1	0	2	20	100.0

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

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

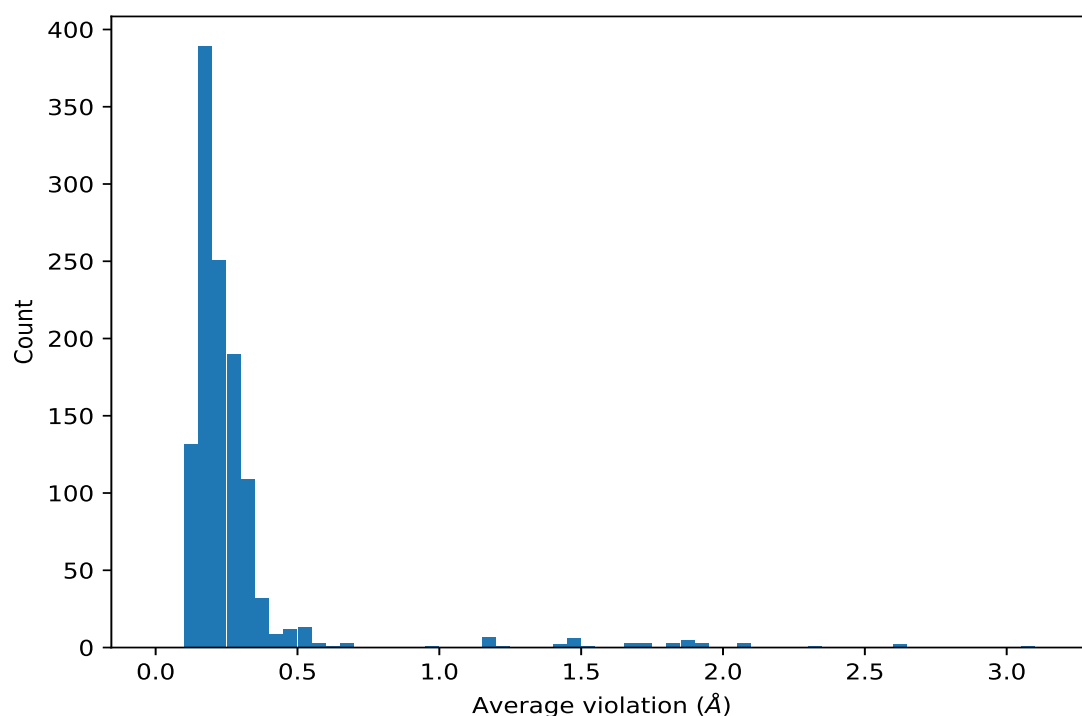
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	20	0.4	0.1	0.44
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	20	0.4	0.1	0.44
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	20	0.27	0.06	0.28
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	19	0.28	0.14	0.25
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	18	0.95	0.18	1.0
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	16	0.22	0.07	0.2
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	14	3.06	0.27	3.02
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	14	2.64	0.15	2.64
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	14	1.94	0.96	1.88
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	14	1.94	0.96	1.88
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	14	1.94	0.96	1.88
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	14	1.51	0.08	1.52
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	14	1.18	0.16	1.19
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	14	0.28	0.08	0.29
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	14	0.28	0.08	0.29
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	14	0.28	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	14	0.28	0.08	0.29
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	13	1.87	0.62	1.69
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	13	1.87	0.62	1.69
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	13	1.87	0.62	1.69
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	13	1.85	1.1	1.52
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	13	1.85	1.1	1.52
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	13	1.81	0.95	1.75
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	13	1.81	0.95	1.75
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	13	1.81	0.95	1.75
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	13	0.35	0.15	0.3
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	13	0.35	0.15	0.3
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	13	0.18	0.03	0.18
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	13	0.18	0.03	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	13	0.18	0.03	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	13	0.18	0.03	0.18
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	12	1.67	1.06	1.54
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	12	1.67	1.06	1.54
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	12	1.67	1.06	1.54
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	12	0.28	0.1	0.28
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	12	0.28	0.1	0.28
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	12	0.26	0.08	0.25
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	12	0.23	0.06	0.22
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	11	2.34	1.33	2.45
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	11	2.09	1.09	2.65
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	11	2.09	1.09	2.65
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	11	2.09	1.09	2.65
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	11	1.74	1.0	1.87
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	11	1.74	1.0	1.87
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	11	1.74	1.0	1.87
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	11	0.24	0.09	0.24
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	11	0.21	0.06	0.22
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	11	0.16	0.03	0.16
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	10	2.61	0.91	2.56
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	10	1.46	0.74	1.66
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	10	0.57	0.19	0.54
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	10	0.57	0.19	0.54
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	10	0.57	0.19	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	10	0.28	0.13	0.26
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	10	0.24	0.09	0.2
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	10	0.24	0.09	0.2
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	10	0.24	0.09	0.2
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	10	0.24	0.09	0.2
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	10	0.24	0.09	0.2
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	10	0.24	0.09	0.2
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	10	0.23	0.07	0.22
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	10	0.23	0.07	0.22
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	10	0.23	0.07	0.22
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	10	0.17	0.05	0.16
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	10	0.17	0.05	0.16
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	10	0.17	0.05	0.16
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	9	1.4	0.94	1.33
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	9	1.4	0.94	1.33
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	9	0.52	0.27	0.51
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	9	0.52	0.27	0.51
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	9	0.52	0.27	0.51
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	9	0.47	0.21	0.48
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	9	0.43	0.23	0.35
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	9	0.43	0.23	0.35
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	9	0.35	0.15	0.3
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	9	0.35	0.17	0.36
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	9	0.32	0.14	0.26
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	9	0.32	0.14	0.26
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	9	0.32	0.14	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	9	0.32	0.13	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	9	0.32	0.13	0.26
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	9	0.25	0.06	0.22
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	9	0.25	0.06	0.22
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	9	0.23	0.1	0.23
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	9	0.21	0.11	0.16
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	9	0.19	0.06	0.17
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	9	0.19	0.06	0.17
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	9	0.18	0.05	0.19
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	9	0.18	0.05	0.19
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	9	0.18	0.05	0.19
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	9	0.15	0.07	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	9	0.12	0.01	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	9	0.12	0.01	0.12
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	8	1.16	0.4	1.09
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	8	1.16	0.4	1.09

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	8	1.16	0.4	1.09
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	8	1.16	0.4	1.09
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	8	1.16	0.4	1.09
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	8	1.16	0.4	1.09
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	8	0.47	0.16	0.5
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	8	0.47	0.16	0.5
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	8	0.31	0.11	0.3
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	8	0.31	0.11	0.3
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	8	0.31	0.11	0.3
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	8	0.29	0.16	0.22
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	8	0.29	0.16	0.22
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	8	0.29	0.1	0.3
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	8	0.29	0.1	0.3
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	8	0.28	0.14	0.18
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	8	0.28	0.14	0.18
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	8	0.27	0.09	0.31
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	8	0.27	0.09	0.31
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	8	0.27	0.09	0.31
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	8	0.25	0.07	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	8	0.25	0.07	0.22
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	8	0.22	0.1	0.2
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	8	0.2	0.08	0.2
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	8	0.2	0.08	0.18
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	8	0.2	0.08	0.18
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	8	0.19	0.05	0.17
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	8	0.19	0.05	0.17
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	8	0.19	0.05	0.17
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	8	0.19	0.05	0.18
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	8	0.18	0.07	0.16
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	8	0.18	0.07	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	8	0.18	0.07	0.16
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	8	0.18	0.07	0.16
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	8	0.18	0.06	0.16
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	8	0.18	0.06	0.16
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	8	0.17	0.07	0.16
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	8	0.16	0.05	0.14
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	8	0.15	0.02	0.16
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	8	0.15	0.02	0.16
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	8	0.15	0.02	0.16
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	8	0.12	0.02	0.12
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	8	0.12	0.02	0.12
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	7	0.29	0.18	0.23
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	7	0.26	0.11	0.25
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	7	0.26	0.11	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	7	0.26	0.11	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	7	0.26	0.11	0.25
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	7	0.24	0.09	0.21
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	7	0.24	0.08	0.23
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	7	0.22	0.09	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	7	0.21	0.06	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	7	0.21	0.06	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	7	0.21	0.06	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	7	0.21	0.06	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	7	0.21	0.06	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	7	0.21	0.06	0.18
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	7	0.21	0.04	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	7	0.21	0.04	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	7	0.21	0.04	0.21
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	7	0.2	0.09	0.19
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	7	0.2	0.09	0.19
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	7	0.2	0.04	0.21
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	7	0.19	0.06	0.15
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	7	0.19	0.11	0.12
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	7	0.17	0.05	0.15
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	7	0.17	0.05	0.15
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	7	0.16	0.03	0.17
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	7	0.16	0.03	0.17
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	7	0.16	0.03	0.17
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	6	1.22	0.7	1.34
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	6	0.36	0.2	0.32
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	6	0.36	0.2	0.32
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	6	0.33	0.12	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	6	0.33	0.12	0.32
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	6	0.33	0.12	0.32
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	6	0.32	0.14	0.3
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	6	0.32	0.14	0.3
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	6	0.32	0.14	0.3
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	6	0.32	0.14	0.3
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	6	0.32	0.14	0.3
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	6	0.32	0.14	0.3
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	6	0.32	0.12	0.27
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	6	0.31	0.24	0.2
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	6	0.31	0.24	0.2
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	6	0.31	0.31	0.14
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	6	0.31	0.31	0.14
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	6	0.31	0.31	0.14
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	6	0.29	0.14	0.23
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	6	0.29	0.14	0.23
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	6	0.28	0.13	0.26
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	6	0.26	0.1	0.26
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	6	0.26	0.1	0.26
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	6	0.26	0.1	0.26
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	6	0.26	0.1	0.26
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	6	0.26	0.1	0.26
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	6	0.26	0.1	0.26
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	6	0.26	0.06	0.28
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	6	0.25	0.18	0.16
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	6	0.25	0.18	0.16
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	6	0.25	0.18	0.16
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	6	0.25	0.18	0.16
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	6	0.25	0.18	0.16
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	6	0.25	0.18	0.16
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	6	0.25	0.07	0.24
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	6	0.25	0.07	0.26
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	6	0.25	0.07	0.26
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	6	0.25	0.07	0.26
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	6	0.25	0.08	0.25
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	6	0.24	0.11	0.2
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	6	0.24	0.1	0.19
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	6	0.24	0.06	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	6	0.24	0.06	0.22
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	6	0.24	0.06	0.22
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	6	0.22	0.1	0.18
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	6	0.22	0.03	0.22
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	6	0.22	0.03	0.22
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	6	0.21	0.08	0.19
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	6	0.21	0.08	0.19
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	6	0.21	0.04	0.2
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	6	0.21	0.04	0.2
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	6	0.21	0.04	0.2
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	6	0.2	0.05	0.2
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	6	0.2	0.05	0.2
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	6	0.2	0.07	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	6	0.2	0.07	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	6	0.2	0.07	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	6	0.2	0.07	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	6	0.2	0.07	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	6	0.2	0.07	0.18
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	6	0.2	0.08	0.18
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	6	0.2	0.08	0.18
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	6	0.2	0.08	0.17
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	6	0.2	0.08	0.17
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	6	0.2	0.08	0.17
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	6	0.19	0.06	0.18
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	6	0.19	0.06	0.18
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	6	0.19	0.06	0.18
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	6	0.17	0.03	0.17
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	6	0.17	0.03	0.17
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	6	0.17	0.03	0.18
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	6	0.17	0.03	0.18
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	6	0.17	0.03	0.18
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	6	0.17	0.06	0.17
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	6	0.17	0.06	0.17
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	6	0.17	0.06	0.17
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	6	0.15	0.04	0.14
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	6	0.14	0.05	0.13
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	6	0.14	0.05	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	6	0.14	0.05	0.13
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	6	0.14	0.03	0.14
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	6	0.14	0.03	0.14
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	5	0.5	0.11	0.57
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	5	0.45	0.03	0.44
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	5	0.45	0.03	0.44
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	5	0.45	0.03	0.44
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	5	0.38	0.03	0.39
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	5	0.38	0.03	0.39
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	5	0.38	0.03	0.39
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	5	0.36	0.21	0.32
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	5	0.36	0.21	0.32
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	5	0.36	0.21	0.32
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	5	0.33	0.1	0.31
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	5	0.33	0.14	0.33
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	5	0.33	0.14	0.33
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	5	0.3	0.13	0.31
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	5	0.29	0.06	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	5	0.29	0.06	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	5	0.29	0.06	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	5	0.29	0.06	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	5	0.29	0.06	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	5	0.29	0.06	0.28
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	5	0.28	0.12	0.27
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	5	0.28	0.12	0.27
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	5	0.28	0.12	0.27
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	5	0.27	0.16	0.23
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	5	0.27	0.14	0.23
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	5	0.26	0.15	0.23
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	5	0.26	0.15	0.23
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	5	0.26	0.15	0.23
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	5	0.26	0.15	0.23
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	5	0.26	0.13	0.2
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	5	0.26	0.13	0.2
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	5	0.26	0.07	0.24
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	5	0.25	0.11	0.22
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	5	0.25	0.11	0.22
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	5	0.25	0.11	0.22
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	5	0.25	0.23	0.14
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	5	0.24	0.03	0.25
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	5	0.23	0.1	0.2
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	5	0.23	0.1	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	5	0.23	0.11	0.21
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	5	0.23	0.08	0.2
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	5	0.23	0.08	0.2
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	5	0.23	0.08	0.2
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	5	0.22	0.03	0.23
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	5	0.22	0.03	0.23
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	5	0.22	0.06	0.2
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	5	0.21	0.05	0.21
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	5	0.21	0.05	0.21
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	5	0.21	0.05	0.21
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	5	0.21	0.04	0.19
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	5	0.21	0.05	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	5	0.21	0.05	0.21
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	5	0.21	0.05	0.21
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	5	0.18	0.05	0.18
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	5	0.18	0.05	0.18
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	5	0.18	0.05	0.18
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	5	0.18	0.08	0.14
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	5	0.18	0.08	0.14
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	5	0.17	0.01	0.18
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	5	0.17	0.01	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	5	0.17	0.01	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	5	0.17	0.01	0.18
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	5	0.17	0.03	0.18
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	5	0.17	0.05	0.15
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	5	0.17	0.04	0.16
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	5	0.17	0.04	0.16
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	5	0.16	0.03	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	5	0.16	0.04	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	5	0.16	0.04	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	5	0.16	0.04	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	5	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	5	0.16	0.04	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	5	0.16	0.04	0.16
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	5	0.16	0.04	0.15
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	5	0.16	0.04	0.15
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	5	0.16	0.04	0.15
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	5	0.16	0.02	0.16
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	5	0.16	0.02	0.16
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	5	0.16	0.03	0.16
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	5	0.16	0.03	0.16
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	5	0.16	0.04	0.16
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	5	0.15	0.05	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	5	0.15	0.03	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	5	0.15	0.03	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	5	0.15	0.03	0.13
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	5	0.14	0.03	0.15
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	5	0.12	0.01	0.11
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	5	0.12	0.01	0.11
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD11	4	0.65	0.39	0.5
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD12	4	0.65	0.39	0.5
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD13	4	0.65	0.39	0.5
(1,926)	1:323:A:ILE:HG21	1:324:A:TYR:HD1	4	0.48	0.53	0.2
(1,926)	1:323:A:ILE:HG22	1:324:A:TYR:HD1	4	0.48	0.53	0.2
(1,926)	1:323:A:ILE:HG23	1:324:A:TYR:HD1	4	0.48	0.53	0.2
(1,1891)	1:225:A:VAL:HA	1:473:A:LYS:HG2	4	0.47	0.03	0.48
(1,17)	1:225:A:VAL:HA	1:226:A:TYR:H	4	0.42	0.06	0.44
(1,1172)	1:348:A:LEU:H	1:348:A:LEU:HG	4	0.34	0.12	0.34
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG2	4	0.34	0.16	0.33
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG3	4	0.34	0.16	0.33
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG2	4	0.34	0.16	0.33
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG3	4	0.34	0.16	0.33
(1,1110)	1:341:A:THR:HB	1:343:A:LEU:HG	4	0.34	0.18	0.28
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD11	4	0.32	0.18	0.34
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD12	4	0.32	0.18	0.34
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD13	4	0.32	0.18	0.34
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB2	4	0.31	0.1	0.35
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB3	4	0.31	0.1	0.35
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD11	4	0.29	0.09	0.29
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD12	4	0.29	0.09	0.29
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD13	4	0.29	0.09	0.29
(1,514)	1:241:A:ASN:HA	1:286:A:ASP:H	4	0.28	0.04	0.28
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB2	4	0.28	0.11	0.28
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB3	4	0.28	0.11	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB2	4	0.28	0.11	0.28
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB3	4	0.28	0.11	0.28
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD11	4	0.26	0.1	0.31
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD12	4	0.26	0.1	0.31
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD13	4	0.26	0.1	0.31
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD21	4	0.26	0.1	0.31
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD22	4	0.26	0.1	0.31
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD23	4	0.26	0.1	0.31
(1,423)	1:277:A:LEU:H	1:279:A:PHE:H	4	0.26	0.03	0.25
(1,227)	1:253:A:LYS:HE2	1:254:A:LEU:HG	4	0.26	0.11	0.22
(1,227)	1:253:A:LYS:HE3	1:254:A:LEU:HG	4	0.26	0.11	0.22
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG2	4	0.26	0.1	0.24
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG3	4	0.26	0.1	0.24
(1,1338)	1:373:A:THR:HB	1:380:A:TYR:HA	4	0.25	0.13	0.23
(1,1233)	1:312:A:CYS:H	1:356:A:PHE:H	4	0.25	0.11	0.2
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB2	4	0.24	0.06	0.26
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB3	4	0.24	0.06	0.26
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG12	4	0.24	0.07	0.22
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG13	4	0.24	0.07	0.22
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG11	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG12	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG13	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG21	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG22	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG23	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG11	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG12	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG13	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG21	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG22	4	0.22	0.07	0.21
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG23	4	0.22	0.07	0.21
(1,865)	1:239:A:ILE:HG21	1:316:A:SER:H	4	0.22	0.08	0.22
(1,865)	1:239:A:ILE:HG22	1:316:A:SER:H	4	0.22	0.08	0.22
(1,865)	1:239:A:ILE:HG23	1:316:A:SER:H	4	0.22	0.08	0.22
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG21	4	0.22	0.08	0.21
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG22	4	0.22	0.08	0.21
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG23	4	0.22	0.08	0.21
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG21	4	0.22	0.08	0.21
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG22	4	0.22	0.08	0.21
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG23	4	0.22	0.08	0.21
(1,448)	1:238:A:ILE:HD11	1:281:A:ILE:HA	4	0.22	0.11	0.18
(1,448)	1:238:A:ILE:HD12	1:281:A:ILE:HA	4	0.22	0.11	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,448)	1:238:A:ILE:HD13	1:281:A:ILE:HA	4	0.22	0.11	0.18
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE2	4	0.2	0.09	0.18
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE3	4	0.2	0.09	0.18
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG2	4	0.2	0.07	0.19
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG3	4	0.2	0.07	0.19
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG21	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG22	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG23	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG21	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG22	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG23	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG21	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG22	4	0.2	0.05	0.19
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG23	4	0.2	0.05	0.19
(1,1835)	1:398:A:ASP:H	1:470:A:LEU:HG	4	0.2	0.08	0.16
(1,281)	1:264:A:HIS:HD2	1:265:A:LEU:HG	4	0.19	0.03	0.2
(1,1548)	1:422:A:ILE:H	1:425:A:LEU:H	4	0.19	0.07	0.17
(1,1564)	1:424:A:SER:HB2	1:426:A:CYS:H	4	0.19	0.05	0.2
(1,1564)	1:424:A:SER:HB3	1:426:A:CYS:H	4	0.19	0.05	0.2
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD2	4	0.19	0.01	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD3	4	0.19	0.01	0.19
(1,1984)	1:310:A:PHE:H	1:476:A:PHE:HE1	4	0.18	0.11	0.12
(1,1409)	1:389:A:GLN:HG2	1:390:A:THR:HA	4	0.18	0.06	0.15
(1,1409)	1:389:A:GLN:HG3	1:390:A:THR:HA	4	0.18	0.06	0.15
(1,1516)	1:403:A:MET:HG2	1:404:A:ALA:H	4	0.18	0.04	0.19
(1,1516)	1:403:A:MET:HG3	1:404:A:ALA:H	4	0.18	0.04	0.19
(1,1795)	1:444:A:THR:HG21	1:446:A:VAL:H	4	0.18	0.07	0.16
(1,1795)	1:444:A:THR:HG22	1:446:A:VAL:H	4	0.18	0.07	0.16
(1,1795)	1:444:A:THR:HG23	1:446:A:VAL:H	4	0.18	0.07	0.16
(1,1845)	1:400:A:LEU:HA	1:470:A:LEU:HG	4	0.18	0.04	0.18
(1,1147)	1:341:A:THR:HG21	1:345:A:CYS:H	4	0.17	0.08	0.14
(1,1147)	1:341:A:THR:HG22	1:345:A:CYS:H	4	0.17	0.08	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1147)	1:341:A:THR:HG23	1:345:A:CYS:H	4	0.17	0.08	0.14
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG21	4	0.17	0.06	0.16
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG22	4	0.17	0.06	0.16
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG23	4	0.17	0.06	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD11	4	0.16	0.05	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD12	4	0.16	0.05	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD13	4	0.16	0.05	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD21	4	0.16	0.05	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD22	4	0.16	0.05	0.16
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD23	4	0.16	0.05	0.16
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD11	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD12	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD13	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD21	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD22	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD23	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD11	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD12	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD13	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD21	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD22	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD23	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD11	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD12	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD13	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD21	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD22	4	0.16	0.06	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD23	4	0.16	0.06	0.15
(1,803)	1:309:A:CYS:HB2	1:310:A:PHE:H	4	0.16	0.04	0.16
(1,803)	1:309:A:CYS:HB3	1:310:A:PHE:H	4	0.16	0.04	0.16
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG21	4	0.16	0.04	0.17
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG22	4	0.16	0.04	0.17
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG23	4	0.16	0.04	0.17
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD11	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD12	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD13	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD21	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD22	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD23	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD11	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD12	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD13	4	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD21	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD22	4	0.16	0.05	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD23	4	0.16	0.05	0.14
(1,697)	1:297:A:LYS:HA	1:299:A:TYR:H	4	0.15	0.04	0.16
(1,1320)	1:248:A:ARG:HD2	1:376:A:GLU:HA	4	0.15	0.04	0.15
(1,1320)	1:248:A:ARG:HD3	1:376:A:GLU:HA	4	0.15	0.04	0.15
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD11	4	0.14	0.05	0.12
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD12	4	0.14	0.05	0.12
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD13	4	0.14	0.05	0.12
(1,914)	1:322:A:ILE:H	1:323:A:ILE:H	4	0.14	0.02	0.15
(1,1892)	1:225:A:VAL:HB	1:473:A:LYS:HA	4	0.14	0.05	0.12
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD11	4	0.14	0.03	0.13
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD12	4	0.14	0.03	0.13
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD13	4	0.14	0.03	0.13
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD21	4	0.14	0.03	0.13
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD22	4	0.14	0.03	0.13
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD23	4	0.14	0.03	0.13
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD2	4	0.13	0.02	0.13
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD3	4	0.13	0.02	0.13
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD2	4	0.13	0.04	0.11
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD3	4	0.13	0.04	0.11
(1,653)	1:295:A:ILE:HG12	1:297:A:LYS:H	4	0.12	0.02	0.13
(1,653)	1:295:A:ILE:HG13	1:297:A:LYS:H	4	0.12	0.02	0.13
(1,162)	1:247:A:ALA:HA	1:249:A:GLU:H	3	0.54	0.19	0.58
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB2	3	0.52	0.01	0.52
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB3	3	0.52	0.01	0.52
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB2	3	0.52	0.11	0.59
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB3	3	0.52	0.11	0.59
(1,969)	1:325:A:GLY:H	1:329:A:GLN:H	3	0.39	0.23	0.39
(1,1954)	1:226:A:TYR:H	1:475:A:VAL:H	3	0.39	0.12	0.31
(1,314)	1:267:A:ALA:HA	1:270:A:LEU:HG	3	0.37	0.25	0.24
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE2	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE2	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE2	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE2	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE2	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE2	3	0.35	0.11	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE3	3	0.35	0.11	0.31
(1,915)	1:322:A:ILE:HG12	1:323:A:ILE:H	3	0.33	0.05	0.3
(1,915)	1:322:A:ILE:HG13	1:323:A:ILE:H	3	0.33	0.05	0.3
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD2	3	0.33	0.14	0.29
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD3	3	0.33	0.14	0.29
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD11	3	0.31	0.17	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD12	3	0.31	0.17	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD13	3	0.31	0.17	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD21	3	0.31	0.17	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD22	3	0.31	0.17	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD23	3	0.31	0.17	0.21
(1,71)	1:232:A:PRO:HA	1:234:A:GLY:H	3	0.31	0.16	0.23
(1,944)	1:247:A:ALA:H	1:327:A:ASP:H	3	0.31	0.08	0.29
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG2	3	0.3	0.1	0.36
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG3	3	0.3	0.1	0.36
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB2	3	0.29	0.1	0.36
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB3	3	0.29	0.1	0.36
(1,795)	1:307:A:MET:HE1	1:309:A:CYS:H	3	0.29	0.09	0.28
(1,795)	1:307:A:MET:HE2	1:309:A:CYS:H	3	0.29	0.09	0.28
(1,795)	1:307:A:MET:HE3	1:309:A:CYS:H	3	0.29	0.09	0.28
(1,1985)	1:310:A:PHE:H	1:476:A:PHE:HZ	3	0.29	0.18	0.17
(1,925)	1:323:A:ILE:HB	1:324:A:TYR:H	3	0.28	0.05	0.31
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG21	3	0.27	0.08	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG22	3	0.27	0.08	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG23	3	0.27	0.08	0.33
(1,933)	1:324:A:TYR:HB3	1:325:A:GLY:H	3	0.27	0.12	0.32
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB1	3	0.27	0.15	0.23
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB2	3	0.27	0.15	0.23
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB3	3	0.27	0.15	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB1	3	0.27	0.15	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB2	3	0.27	0.15	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB3	3	0.27	0.15	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD11	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD12	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD13	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD21	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD22	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD23	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD11	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD12	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD13	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD21	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD22	3	0.27	0.07	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD23	3	0.27	0.07	0.3
(1,1356)	1:373:A:THR:HB	1:381:A:LEU:HG	3	0.26	0.1	0.24
(1,1633)	1:430:A:ARG:HG2	1:431:A:GLU:H	3	0.26	0.05	0.29
(1,1633)	1:430:A:ARG:HG3	1:431:A:GLU:H	3	0.26	0.05	0.29
(1,1315)	1:373:A:THR:HB	1:374:A:ASP:HA	3	0.26	0.09	0.21
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG21	3	0.25	0.08	0.29
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG22	3	0.25	0.08	0.29
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG23	3	0.25	0.08	0.29
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG2	3	0.24	0.15	0.15
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG3	3	0.24	0.15	0.15
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG2	3	0.24	0.15	0.15
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG3	3	0.24	0.15	0.15
(1,912)	1:322:A:ILE:HB	1:323:A:ILE:H	3	0.24	0.07	0.25
(1,1719)	1:439:A:ILE:HG21	1:441:A:THR:H	3	0.24	0.06	0.23
(1,1719)	1:439:A:ILE:HG22	1:441:A:THR:H	3	0.24	0.06	0.23
(1,1719)	1:439:A:ILE:HG23	1:441:A:THR:H	3	0.24	0.06	0.23
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB2	3	0.24	0.08	0.25
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB3	3	0.24	0.08	0.25
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB2	3	0.24	0.08	0.25
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB3	3	0.24	0.08	0.25
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD2	3	0.23	0.07	0.23
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD3	3	0.23	0.07	0.23
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB2	3	0.23	0.07	0.2
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB3	3	0.23	0.07	0.2
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD11	3	0.22	0.02	0.22
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD12	3	0.22	0.02	0.22
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD13	3	0.22	0.02	0.22
(1,1671)	1:435:A:ARG:HG2	1:436:A:GLY:H	3	0.22	0.04	0.25
(1,1671)	1:435:A:ARG:HG3	1:436:A:GLY:H	3	0.22	0.04	0.25
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG21	3	0.21	0.05	0.22
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG22	3	0.21	0.05	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG23	3	0.21	0.05	0.22
(1,828)	1:311:A:ILE:HD11	1:312:A:CYS:H	3	0.21	0.08	0.2
(1,828)	1:311:A:ILE:HD12	1:312:A:CYS:H	3	0.21	0.08	0.2
(1,828)	1:311:A:ILE:HD13	1:312:A:CYS:H	3	0.21	0.08	0.2
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA2	3	0.21	0.06	0.23
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA3	3	0.21	0.06	0.23
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG2	3	0.2	0.05	0.19
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG3	3	0.2	0.05	0.19
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG2	3	0.2	0.05	0.19
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG3	3	0.2	0.05	0.19
(1,1858)	1:469:A:THR:HA	1:470:A:LEU:HA	3	0.2	0.01	0.2
(1,217)	1:251:A:VAL:HG21	1:254:A:LEU:HG	3	0.19	0.03	0.19
(1,217)	1:251:A:VAL:HG22	1:254:A:LEU:HG	3	0.19	0.03	0.19
(1,217)	1:251:A:VAL:HG23	1:254:A:LEU:HG	3	0.19	0.03	0.19
(1,898)	1:320:A:LYS:HB2	1:322:A:ILE:H	3	0.19	0.04	0.17
(1,898)	1:320:A:LYS:HB3	1:322:A:ILE:H	3	0.19	0.04	0.17
(1,422)	1:275:A:GLU:HA	1:279:A:PHE:H	3	0.19	0.06	0.16
(1,1748)	1:356:A:PHE:HE1	1:443:A:LEU:H	3	0.19	0.04	0.18
(1,885)	1:319:A:ASP:H	1:322:A:ILE:H	3	0.19	0.04	0.21
(1,7)	1:224:A:LYS:HB3	1:225:A:VAL:HB	3	0.18	0.05	0.21
(1,550)	1:287:A:CYS:HB2	1:291:A:GLN:H	3	0.18	0.02	0.19
(1,550)	1:287:A:CYS:HB3	1:291:A:GLN:H	3	0.18	0.02	0.19
(1,910)	1:322:A:ILE:HA	1:323:A:ILE:H	3	0.18	0.01	0.19
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB2	3	0.18	0.05	0.15
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB3	3	0.18	0.05	0.15
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB2	3	0.18	0.05	0.15
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB3	3	0.18	0.05	0.15
(1,1816)	1:467:A:THR:HA	1:468:A:PHE:H	3	0.18	0.01	0.18
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD12	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD12	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD12	3	0.18	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD12	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD12	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD11	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD12	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD13	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD21	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD22	3	0.18	0.04	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD23	3	0.18	0.04	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD11	3	0.18	0.05	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD12	3	0.18	0.05	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD13	3	0.18	0.05	0.19
(1,706)	1:298:A:ILE:HD11	1:299:A:TYR:HE1	3	0.17	0.03	0.16
(1,706)	1:298:A:ILE:HD12	1:299:A:TYR:HE1	3	0.17	0.03	0.16
(1,706)	1:298:A:ILE:HD13	1:299:A:TYR:HE1	3	0.17	0.03	0.16
(1,1482)	1:400:A:LEU:HG	1:401:A:LEU:H	3	0.17	0.03	0.19
(1,987)	1:324:A:TYR:HA	1:330:A:GLU:HA	3	0.17	0.06	0.13
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE2	3	0.17	0.05	0.15
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE3	3	0.17	0.05	0.15
(1,1255)	1:357:A:ILE:HG21	1:359:A:ALA:HA	3	0.17	0.02	0.17
(1,1255)	1:357:A:ILE:HG22	1:359:A:ALA:HA	3	0.17	0.02	0.17
(1,1255)	1:357:A:ILE:HG23	1:359:A:ALA:HA	3	0.17	0.02	0.17
(1,1298)	1:370:A:PRO:HB2	1:371:A:VAL:H	3	0.17	0.05	0.14
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA2	3	0.17	0.05	0.15
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA3	3	0.17	0.05	0.15
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA2	3	0.17	0.05	0.15
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA3	3	0.17	0.05	0.15
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB1	3	0.17	0.07	0.13
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB2	3	0.17	0.07	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB3	3	0.17	0.07	0.13
(1,1933)	1:470:A:LEU:HD11	1:474:A:LEU:H	3	0.17	0.04	0.17
(1,1933)	1:470:A:LEU:HD12	1:474:A:LEU:H	3	0.17	0.04	0.17
(1,1933)	1:470:A:LEU:HD13	1:474:A:LEU:H	3	0.17	0.04	0.17
(1,1072)	1:336:A:LEU:HG	1:337:A:THR:H	3	0.16	0.05	0.13
(1,1236)	1:314:A:ILE:H	1:356:A:PHE:H	3	0.16	0.04	0.17
(1,1312)	1:248:A:ARG:HG2	1:373:A:THR:HB	3	0.16	0.06	0.13
(1,1312)	1:248:A:ARG:HG3	1:373:A:THR:HB	3	0.16	0.06	0.13
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG21	3	0.16	0.05	0.17
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG22	3	0.16	0.05	0.17
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG23	3	0.16	0.05	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG21	3	0.16	0.05	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG22	3	0.16	0.05	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG23	3	0.16	0.05	0.17
(1,1267)	1:360:A:ALA:HB1	1:361:A:GLN:HA	3	0.16	0.04	0.17
(1,1267)	1:360:A:ALA:HB2	1:361:A:GLN:HA	3	0.16	0.04	0.17
(1,1267)	1:360:A:ALA:HB3	1:361:A:GLN:HA	3	0.16	0.04	0.17
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD11	3	0.16	0.03	0.15
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD12	3	0.16	0.03	0.15
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD13	3	0.16	0.03	0.15
(1,276)	1:258:A:ARG:H	1:259:A:ASP:HA	3	0.16	0.04	0.16
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD11	3	0.15	0.02	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD12	3	0.15	0.02	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD13	3	0.15	0.02	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD21	3	0.15	0.02	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD22	3	0.15	0.02	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD23	3	0.15	0.02	0.17
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD11	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD12	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD13	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD21	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD22	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD23	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD11	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD12	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD13	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD21	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD22	3	0.15	0.03	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD23	3	0.15	0.03	0.14
(1,1079)	1:337:A:THR:HG21	1:338:A:SER:H	3	0.15	0.02	0.15
(1,1079)	1:337:A:THR:HG22	1:338:A:SER:H	3	0.15	0.02	0.15
(1,1079)	1:337:A:THR:HG23	1:338:A:SER:H	3	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,161)	1:247:A:ALA:HB1	1:249:A:GLU:H	3	0.14	0.02	0.15
(1,161)	1:247:A:ALA:HB2	1:249:A:GLU:H	3	0.14	0.02	0.15
(1,161)	1:247:A:ALA:HB3	1:249:A:GLU:H	3	0.14	0.02	0.15
(1,413)	1:276:A:GLU:H	1:278:A:HIS:H	3	0.14	0.04	0.12
(1,501)	1:240:A:ASN:HB2	1:284:A:HIS:H	3	0.14	0.03	0.12
(1,501)	1:240:A:ASN:HB3	1:284:A:HIS:H	3	0.14	0.03	0.12
(1,801)	1:309:A:CYS:HB2	1:310:A:PHE:H	3	0.14	0.03	0.16
(1,627)	1:293:A:TYR:H	1:295:A:ILE:H	3	0.14	0.0	0.14
(1,1103)	1:340:A:PHE:HB2	1:341:A:THR:H	3	0.13	0.01	0.14
(1,1103)	1:340:A:PHE:HB3	1:341:A:THR:H	3	0.13	0.01	0.14
(1,2017)	1:277:A:LEU:HD11	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,2017)	1:277:A:LEU:HD12	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,2017)	1:277:A:LEU:HD13	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,2017)	1:277:A:LEU:HD21	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,2017)	1:277:A:LEU:HD22	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,2017)	1:277:A:LEU:HD23	1:479:A:ASP:H	3	0.13	0.03	0.12
(1,127)	1:244:A:PHE:HA	1:245:A:ALA:H	3	0.13	0.02	0.14
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG2	3	0.13	0.01	0.12
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG3	3	0.13	0.01	0.12
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB1	3	0.13	0.01	0.13
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB2	3	0.13	0.01	0.13
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB3	3	0.13	0.01	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD11	3	0.12	0.02	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD12	3	0.12	0.02	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD13	3	0.12	0.02	0.13
(1,1154)	1:344:A:LYS:HG2	1:345:A:CYS:H	3	0.12	0.01	0.12
(1,494)	1:238:A:ILE:H	1:284:A:HIS:HD2	3	0.12	0.01	0.13
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB2	3	0.12	0.02	0.11
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB3	3	0.12	0.02	0.11
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB2	3	0.12	0.02	0.11
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB3	3	0.12	0.02	0.11
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB2	3	0.12	0.02	0.11
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB3	3	0.12	0.02	0.11
(1,1149)	1:341:A:THR:HB	1:345:A:CYS:H	2	0.61	0.08	0.61
(1,1771)	1:443:A:LEU:H	1:444:A:THR:H	2	0.53	0.18	0.53
(1,1375)	1:380:A:TYR:HD1	1:381:A:LEU:HA	2	0.52	0.13	0.52
(1,1190)	1:348:A:LEU:HA	1:351:A:LYS:H	2	0.52	0.24	0.52
(1,538)	1:288:A:THR:HA	1:290:A:GLU:H	2	0.5	0.3	0.5
(1,1379)	1:381:A:LEU:HA	1:381:A:LEU:HG	2	0.48	0.01	0.48
(1,968)	1:324:A:TYR:HA	1:329:A:GLN:H	2	0.45	0.03	0.45
(1,123)	1:243:A:ASN:HA	1:244:A:PHE:H	2	0.42	0.04	0.42
(1,319)	1:269:A:ALA:HB1	1:270:A:LEU:HG	2	0.41	0.18	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,319)	1:269:A:ALA:HB2	1:270:A:LEU:HG	2	0.41	0.18	0.41
(1,319)	1:269:A:ALA:HB3	1:270:A:LEU:HG	2	0.41	0.18	0.41
(1,289)	1:265:A:LEU:HB3	1:266:A:ASP:H	2	0.39	0.09	0.39
(1,1536)	1:422:A:ILE:HB	1:423:A:GLN:HA	2	0.39	0.06	0.39
(1,940)	1:246:A:LYS:HB2	1:327:A:ASP:HA	2	0.38	0.02	0.38
(1,940)	1:246:A:LYS:HB3	1:327:A:ASP:HA	2	0.38	0.02	0.38
(1,433)	1:235:A:TYR:HA	1:280:A:GLU:H	2	0.38	0.26	0.38
(1,432)	1:234:A:GLY:H	1:280:A:GLU:H	2	0.34	0.01	0.34
(1,387)	1:273:A:THR:HA	1:276:A:GLU:H	2	0.32	0.02	0.32
(1,1018)	1:333:A:ILE:HG21	1:335:A:GLU:H	2	0.32	0.2	0.32
(1,1018)	1:333:A:ILE:HG22	1:335:A:GLU:H	2	0.32	0.2	0.32
(1,1018)	1:333:A:ILE:HG23	1:335:A:GLU:H	2	0.32	0.2	0.32
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG21	2	0.32	0.03	0.32
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG22	2	0.32	0.03	0.32
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG23	2	0.32	0.03	0.32
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG2	2	0.32	0.08	0.32
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG2	2	0.32	0.08	0.32
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG2	2	0.32	0.08	0.32
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG3	2	0.32	0.08	0.32
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG3	2	0.32	0.08	0.32
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG3	2	0.32	0.08	0.32
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB2	2	0.32	0.16	0.32
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB3	2	0.32	0.16	0.32
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB2	2	0.32	0.16	0.32
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB3	2	0.32	0.16	0.32
(1,163)	1:248:A:ARG:HG2	1:249:A:GLU:H	2	0.31	0.08	0.31
(1,163)	1:248:A:ARG:HG3	1:249:A:GLU:H	2	0.31	0.08	0.31
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB2	2	0.3	0.13	0.3
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB3	2	0.3	0.13	0.3
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD11	2	0.3	0.16	0.3
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD12	2	0.3	0.16	0.3
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD13	2	0.3	0.16	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD11	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD12	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD13	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD21	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD22	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD23	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD11	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD12	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD13	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD21	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD22	2	0.3	0.1	0.3
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD23	2	0.3	0.1	0.3
(1,903)	1:322:A:ILE:H	1:322:A:ILE:HG13	2	0.29	0.05	0.29
(1,705)	1:298:A:ILE:HG21	1:299:A:TYR:HE1	2	0.27	0.05	0.27
(1,705)	1:298:A:ILE:HG22	1:299:A:TYR:HE1	2	0.27	0.05	0.27
(1,705)	1:298:A:ILE:HG23	1:299:A:TYR:HE1	2	0.27	0.05	0.27
(1,291)	1:265:A:LEU:HB2	1:266:A:ASP:H	2	0.26	0.02	0.26
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA2	2	0.26	0.16	0.26
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA3	2	0.26	0.16	0.26
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA2	2	0.26	0.16	0.26
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA3	2	0.26	0.16	0.26
(1,154)	1:247:A:ALA:HB1	1:248:A:ARG:H	2	0.26	0.02	0.26
(1,154)	1:247:A:ALA:HB2	1:248:A:ARG:H	2	0.26	0.02	0.26
(1,154)	1:247:A:ALA:HB3	1:248:A:ARG:H	2	0.26	0.02	0.26
(1,224)	1:251:A:VAL:HG11	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,224)	1:251:A:VAL:HG12	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,224)	1:251:A:VAL:HG13	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,224)	1:251:A:VAL:HG21	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,224)	1:251:A:VAL:HG22	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,224)	1:251:A:VAL:HG23	1:254:A:LEU:HG	2	0.26	0.07	0.26
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD11	2	0.26	0.15	0.26
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD12	2	0.26	0.15	0.26
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD13	2	0.26	0.15	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD11	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD12	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD13	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD21	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD22	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD23	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD11	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD12	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD13	2	0.26	0.0	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD21	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD22	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD23	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD11	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD12	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD13	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD21	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD22	2	0.26	0.0	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD23	2	0.26	0.0	0.26
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG11	2	0.26	0.06	0.26
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG12	2	0.26	0.06	0.26
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG13	2	0.26	0.06	0.26
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD11	2	0.25	0.02	0.25
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD12	2	0.25	0.02	0.25
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD13	2	0.25	0.02	0.25
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD21	2	0.25	0.02	0.25
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD22	2	0.25	0.02	0.25
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD23	2	0.25	0.02	0.25
(1,465)	1:280:A:GLU:HB3	1:281:A:ILE:H	2	0.25	0.03	0.25
(1,1019)	1:333:A:ILE:H	1:335:A:GLU:H	2	0.25	0.12	0.25
(1,1022)	1:334:A:TYR:HB2	1:335:A:GLU:H	2	0.25	0.09	0.25
(1,1126)	1:341:A:THR:H	1:344:A:LYS:H	2	0.25	0.12	0.25
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD11	2	0.25	0.06	0.25
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD12	2	0.25	0.06	0.25
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD13	2	0.25	0.06	0.25
(1,325)	1:238:A:ILE:HD11	1:271:A:THR:HB	2	0.24	0.04	0.24
(1,325)	1:238:A:ILE:HD12	1:271:A:THR:HB	2	0.24	0.04	0.24
(1,325)	1:238:A:ILE:HD13	1:271:A:THR:HB	2	0.24	0.04	0.24
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB2	2	0.24	0.03	0.24
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB3	2	0.24	0.03	0.24
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB2	2	0.24	0.03	0.24
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB3	2	0.24	0.03	0.24
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB2	2	0.24	0.03	0.24
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB3	2	0.24	0.03	0.24
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD11	2	0.24	0.02	0.24
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD12	2	0.24	0.02	0.24
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD13	2	0.24	0.02	0.24
(1,2012)	1:277:A:LEU:HD11	1:478:A:SER:HA	2	0.24	0.1	0.24
(1,2012)	1:277:A:LEU:HD12	1:478:A:SER:HA	2	0.24	0.1	0.24
(1,2012)	1:277:A:LEU:HD13	1:478:A:SER:HA	2	0.24	0.1	0.24
(1,2012)	1:277:A:LEU:HD21	1:478:A:SER:HA	2	0.24	0.1	0.24
(1,2012)	1:277:A:LEU:HD22	1:478:A:SER:HA	2	0.24	0.1	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2012)	1:277:A:LEU:HD23	1:478:A:SER:HA	2	0.24	0.1	0.24
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB2	2	0.24	0.07	0.24
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB3	2	0.24	0.07	0.24
(1,346)	1:271:A:THR:H	1:273:A:THR:H	2	0.24	0.08	0.24
(1,534)	1:288:A:THR:HB	1:289:A:VAL:H	2	0.24	0.05	0.24
(1,523)	1:239:A:ILE:HG21	1:287:A:CYS:H	2	0.23	0.08	0.23
(1,523)	1:239:A:ILE:HG22	1:287:A:CYS:H	2	0.23	0.08	0.23
(1,523)	1:239:A:ILE:HG23	1:287:A:CYS:H	2	0.23	0.08	0.23
(1,935)	1:288:A:THR:HG21	1:326:A:THR:H	2	0.23	0.07	0.23
(1,935)	1:288:A:THR:HG22	1:326:A:THR:H	2	0.23	0.07	0.23
(1,935)	1:288:A:THR:HG23	1:326:A:THR:H	2	0.23	0.07	0.23
(1,1192)	1:349:A:ALA:HA	1:351:A:LYS:H	2	0.23	0.12	0.23
(1,1347)	1:380:A:TYR:H	1:380:A:TYR:HD1	2	0.23	0.08	0.23
(1,1770)	1:443:A:LEU:HG	1:444:A:THR:H	2	0.23	0.01	0.23
(1,651)	1:294:A:GLU:H	1:297:A:LYS:H	2	0.22	0.02	0.22
(1,932)	1:324:A:TYR:HA	1:325:A:GLY:H	2	0.22	0.04	0.22
(1,1063)	1:334:A:TYR:HA	1:337:A:THR:H	2	0.22	0.08	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG21	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG22	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG23	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG21	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG22	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG23	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG21	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG22	2	0.22	0.01	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG23	2	0.22	0.01	0.22
(1,431)	1:279:A:PHE:H	1:279:A:PHE:HD1	2	0.22	0.1	0.22
(1,990)	1:329:A:GLN:HB2	1:330:A:GLU:H	2	0.21	0.07	0.21
(1,990)	1:329:A:GLN:HB3	1:330:A:GLU:H	2	0.21	0.07	0.21
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD11	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD12	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD13	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD11	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD12	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD13	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD11	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD12	2	0.21	0.03	0.21
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD13	2	0.21	0.03	0.21
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG11	2	0.2	0.04	0.2
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG12	2	0.2	0.04	0.2
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG13	2	0.2	0.04	0.2
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG21	2	0.2	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG22	2	0.2	0.04	0.2
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG23	2	0.2	0.04	0.2
(1,1302)	1:370:A:PRO:HB2	1:371:A:VAL:HA	2	0.2	0.02	0.2
(1,38)	1:228:A:MET:HA	1:229:A:LYS:H	2	0.2	0.02	0.2
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE2	2	0.2	0.06	0.2
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE3	2	0.2	0.06	0.2
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD2	2	0.2	0.01	0.2
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD3	2	0.2	0.01	0.2
(1,175)	1:249:A:GLU:HB2	1:250:A:LYS:H	2	0.2	0.08	0.2
(1,175)	1:249:A:GLU:HB3	1:250:A:LYS:H	2	0.2	0.08	0.2
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD11	2	0.2	0.04	0.2
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD12	2	0.2	0.04	0.2
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD13	2	0.2	0.04	0.2
(1,870)	1:317:A:HIS:HA	1:318:A:GLY:H	2	0.2	0.09	0.2
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB2	2	0.2	0.06	0.2
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB3	2	0.2	0.06	0.2
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB2	2	0.2	0.01	0.2
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB3	2	0.2	0.01	0.2
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB2	2	0.2	0.02	0.2
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB3	2	0.2	0.02	0.2
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD11	2	0.19	0.04	0.19
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD12	2	0.19	0.04	0.19
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD13	2	0.19	0.04	0.19
(1,1822)	1:399:A:PHE:H	1:469:A:THR:H	2	0.19	0.01	0.19
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG12	2	0.18	0.02	0.18
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG13	2	0.18	0.02	0.18
(1,146)	1:245:A:ALA:H	1:247:A:ALA:H	2	0.18	0.05	0.18
(1,187)	1:247:A:ALA:HB1	1:251:A:VAL:H	2	0.18	0.05	0.18
(1,187)	1:247:A:ALA:HB2	1:251:A:VAL:H	2	0.18	0.05	0.18
(1,187)	1:247:A:ALA:HB3	1:251:A:VAL:H	2	0.18	0.05	0.18
(1,1085)	1:337:A:THR:H	1:339:A:GLN:H	2	0.18	0.01	0.18
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG2	2	0.18	0.04	0.18
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG3	2	0.18	0.04	0.18
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB2	2	0.18	0.03	0.18
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB3	2	0.18	0.03	0.18
(1,211)	1:247:A:ALA:HB1	1:254:A:LEU:HG	2	0.18	0.06	0.18
(1,211)	1:247:A:ALA:HB2	1:254:A:LEU:HG	2	0.18	0.06	0.18
(1,211)	1:247:A:ALA:HB3	1:254:A:LEU:HG	2	0.18	0.06	0.18
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB2	2	0.18	0.03	0.18
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB3	2	0.18	0.03	0.18
(1,714)	1:298:A:ILE:H	1:300:A:GLN:H	2	0.18	0.0	0.18
(1,931)	1:324:A:TYR:HB2	1:325:A:GLY:H	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1820)	1:397:A:ALA:HB1	1:469:A:THR:HB	2	0.18	0.0	0.18
(1,1820)	1:397:A:ALA:HB2	1:469:A:THR:HB	2	0.18	0.0	0.18
(1,1820)	1:397:A:ALA:HB3	1:469:A:THR:HB	2	0.18	0.0	0.18
(1,1983)	1:228:A:MET:HE1	1:476:A:PHE:HE1	2	0.18	0.03	0.18
(1,1983)	1:228:A:MET:HE2	1:476:A:PHE:HE1	2	0.18	0.03	0.18
(1,1983)	1:228:A:MET:HE3	1:476:A:PHE:HE1	2	0.18	0.03	0.18
(1,1565)	1:424:A:SER:HA	1:426:A:CYS:H	2	0.17	0.06	0.17
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB2	2	0.17	0.01	0.17
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB3	2	0.17	0.01	0.17
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB2	2	0.17	0.01	0.17
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB3	2	0.17	0.01	0.17
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB2	2	0.17	0.01	0.17
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB3	2	0.17	0.01	0.17
(1,1759)	1:439:A:ILE:HA	1:443:A:LEU:H	2	0.17	0.04	0.17
(1,1980)	1:474:A:LEU:HD11	1:475:A:VAL:H	2	0.17	0.04	0.17
(1,1980)	1:474:A:LEU:HD12	1:475:A:VAL:H	2	0.17	0.04	0.17
(1,1980)	1:474:A:LEU:HD13	1:475:A:VAL:H	2	0.17	0.04	0.17
(1,1807)	1:443:A:LEU:HD11	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1807)	1:443:A:LEU:HD12	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1807)	1:443:A:LEU:HD13	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1807)	1:443:A:LEU:HD21	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1807)	1:443:A:LEU:HD22	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1807)	1:443:A:LEU:HD23	1:467:A:THR:H	2	0.16	0.06	0.16
(1,1888)	1:224:A:LYS:HA	1:473:A:LYS:H	2	0.16	0.01	0.16
(1,1942)	1:473:A:LYS:HE2	1:474:A:LEU:H	2	0.16	0.06	0.16
(1,1942)	1:473:A:LYS:HE3	1:474:A:LEU:H	2	0.16	0.06	0.16
(1,148)	1:246:A:LYS:HB2	1:247:A:ALA:H	2	0.16	0.02	0.16
(1,148)	1:246:A:LYS:HB3	1:247:A:ALA:H	2	0.16	0.02	0.16
(1,48)	1:229:A:LYS:HG2	1:230:A:SER:H	2	0.16	0.04	0.16
(1,48)	1:229:A:LYS:HG3	1:230:A:SER:H	2	0.16	0.04	0.16
(1,469)	1:280:A:GLU:HB3	1:281:A:ILE:HA	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG22	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG22	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG22	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG22	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG22	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG21	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG22	2	0.16	0.05	0.16
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG23	2	0.16	0.05	0.16
(1,709)	1:299:A:TYR:H	1:299:A:TYR:HE1	2	0.16	0.02	0.16
(1,1092)	1:339:A:GLN:H	1:340:A:PHE:HA	2	0.16	0.01	0.16
(1,1232)	1:311:A:ILE:HG21	1:356:A:PHE:HE1	2	0.16	0.05	0.16
(1,1232)	1:311:A:ILE:HG22	1:356:A:PHE:HE1	2	0.16	0.05	0.16
(1,1232)	1:311:A:ILE:HG23	1:356:A:PHE:HE1	2	0.16	0.05	0.16
(1,1640)	1:273:A:THR:HG21	1:433:A:CYS:H	2	0.16	0.02	0.16
(1,1640)	1:273:A:THR:HG22	1:433:A:CYS:H	2	0.16	0.02	0.16
(1,1640)	1:273:A:THR:HG23	1:433:A:CYS:H	2	0.16	0.02	0.16
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA2	2	0.16	0.05	0.16
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG2	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG3	2	0.16	0.05	0.16
(1,491)	1:238:A:ILE:HD11	1:283:A:PRO:HA	2	0.15	0.01	0.15
(1,491)	1:238:A:ILE:HD12	1:283:A:PRO:HA	2	0.15	0.01	0.15
(1,491)	1:238:A:ILE:HD13	1:283:A:PRO:HA	2	0.15	0.01	0.15
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD21	2	0.15	0.04	0.15
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD22	2	0.15	0.04	0.15
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD23	2	0.15	0.04	0.15
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD21	2	0.15	0.04	0.15
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD22	2	0.15	0.04	0.15
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD23	2	0.15	0.04	0.15
(1,1098)	1:340:A:PHE:H	1:341:A:THR:HA	2	0.15	0.0	0.15
(1,118)	1:241:A:ASN:HA	1:243:A:ASN:H	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD11	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD12	2	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD13	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD11	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD12	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD13	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD11	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD12	2	0.15	0.03	0.15
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD13	2	0.15	0.03	0.15
(1,1250)	1:357:A:ILE:HA	1:358:A:GLN:H	2	0.15	0.02	0.15
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB2	2	0.14	0.03	0.14
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB3	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG21	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG22	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG23	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG21	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG22	2	0.14	0.03	0.14
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG23	2	0.14	0.03	0.14
(1,268)	1:257:A:ILE:HB	1:258:A:ARG:H	2	0.14	0.02	0.14
(1,930)	1:324:A:TYR:HD1	1:325:A:GLY:H	2	0.14	0.02	0.14
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB2	2	0.14	0.03	0.14
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB3	2	0.14	0.03	0.14
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB2	2	0.14	0.03	0.14
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB3	2	0.14	0.03	0.14
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB2	2	0.14	0.03	0.14
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB3	2	0.14	0.03	0.14
(1,1058)	1:296:A:LEU:HD11	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1058)	1:296:A:LEU:HD12	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1058)	1:296:A:LEU:HD13	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1058)	1:296:A:LEU:HD21	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1058)	1:296:A:LEU:HD22	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1058)	1:296:A:LEU:HD23	1:337:A:THR:HB	2	0.14	0.02	0.14
(1,1489)	1:356:A:PHE:HA	1:402:A:GLY:H	2	0.14	0.02	0.14
(1,548)	1:287:A:CYS:HA	1:291:A:GLN:H	2	0.14	0.01	0.14
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD2	2	0.14	0.04	0.14
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD3	2	0.14	0.04	0.14
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE1	2	0.14	0.02	0.14
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE2	2	0.14	0.02	0.14
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE3	2	0.14	0.02	0.14
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE1	2	0.14	0.02	0.14
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE2	2	0.14	0.02	0.14
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE3	2	0.14	0.02	0.14
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD2	2	0.14	0.02	0.14
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD3	2	0.14	0.02	0.14

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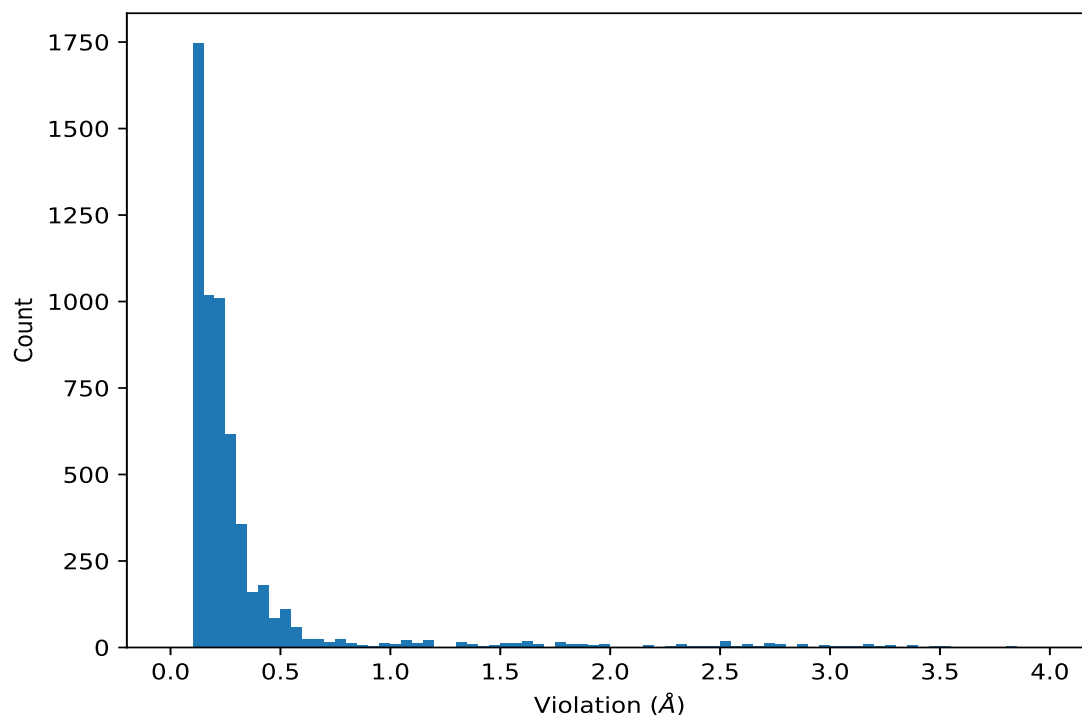
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1373)	1:380:A:TYR:HA	1:381:A:LEU:HG	2	0.14	0.02	0.14
(1,1587)	1:427:A:GLN:HB2	1:428:A:SER:H	2	0.14	0.02	0.14
(1,1587)	1:427:A:GLN:HB3	1:428:A:SER:H	2	0.14	0.02	0.14
(1,1854)	1:469:A:THR:HG21	1:470:A:LEU:H	2	0.14	0.04	0.14
(1,1854)	1:469:A:THR:HG22	1:470:A:LEU:H	2	0.14	0.04	0.14
(1,1854)	1:469:A:THR:HG23	1:470:A:LEU:H	2	0.14	0.04	0.14
(1,267)	1:257:A:ILE:HA	1:258:A:ARG:H	2	0.13	0.01	0.13
(1,1043)	1:335:A:GLU:H	1:336:A:LEU:HA	2	0.13	0.01	0.13
(1,435)	1:235:A:TYR:HB2	1:280:A:GLU:HB3	2	0.12	0.02	0.12
(1,435)	1:235:A:TYR:HB3	1:280:A:GLU:HB3	2	0.12	0.02	0.12
(1,1016)	1:334:A:TYR:HB2	1:334:A:TYR:HE1	2	0.12	0.01	0.12
(1,1224)	1:354:A:VAL:HG21	1:355:A:PHE:H	2	0.12	0.02	0.12
(1,1224)	1:354:A:VAL:HG22	1:355:A:PHE:H	2	0.12	0.02	0.12
(1,1224)	1:354:A:VAL:HG23	1:355:A:PHE:H	2	0.12	0.02	0.12
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG2	2	0.12	0.02	0.12
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG3	2	0.12	0.02	0.12
(1,343)	1:269:A:ALA:HA	1:273:A:THR:H	2	0.12	0.02	0.12
(1,886)	1:319:A:ASP:H	1:322:A:ILE:HB	2	0.12	0.0	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG21	2	0.12	0.0	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG22	2	0.12	0.0	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG23	2	0.12	0.0	0.12
(1,1280)	1:369:A:ILE:H	1:369:A:ILE:HB	2	0.12	0.0	0.12
(1,1394)	1:384:A:ASP:H	1:385:A:LEU:HA	2	0.12	0.0	0.12
(1,1972)	1:473:A:LYS:HE2	1:475:A:VAL:H	2	0.12	0.0	0.12
(1,1972)	1:473:A:LYS:HE3	1:475:A:VAL:H	2	0.12	0.0	0.12
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE2	2	0.12	0.02	0.12
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE3	2	0.12	0.02	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD11	2	0.12	0.0	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD12	2	0.12	0.0	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD13	2	0.12	0.0	0.12
(1,762)	1:300:A:GLN:H	1:303:A:ASP:H	2	0.11	0.01	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD11	2	0.11	0.0	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD12	2	0.11	0.0	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD13	2	0.11	0.0	0.11
(1,1044)	1:335:A:GLU:H	1:336:A:LEU:HG	2	0.11	0.0	0.11
(1,1286)	1:369:A:ILE:HG13	1:370:A:PRO:HD2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	6	3.99
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	7	3.93
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	15	3.84
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	4	3.83
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	4	3.83
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	7	3.7
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	15	3.68
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	6	3.64
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	16	3.55
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	16	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	16	3.55
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	17	3.52
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	19	3.47
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	19	3.47
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	19	3.47
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	13	3.37
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	13	3.37
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	13	3.37
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	7	3.37
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	18	3.37
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	12	3.36
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	17	3.33
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	3	3.32
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	1	3.29
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	19	3.27
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	19	3.27
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	19	3.27
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	11	3.26
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	11	3.26
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	16	3.2
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	16	3.2
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	16	3.2
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	19	3.18
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	19	3.18
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	19	3.18
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	12	3.17
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	12	3.17
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	12	3.17
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	8	3.16
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	8	3.16
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	8	3.16
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	15	3.11
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	15	3.11
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	15	3.11
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	11	3.11
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	11	3.11
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	1	3.06
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	1	3.06
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	1	3.06
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	12	3.05
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	12	3.05
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	12	3.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	11	3.03
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	14	3.02
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	1	2.97
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	1	2.97
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	1	2.97
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	17	2.97
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	13	2.97
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	13	2.95
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	13	2.95
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	13	2.95
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	2	2.91
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	16	2.9
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	16	2.9
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	16	2.9
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	9	2.88
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	9	2.88
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	13	2.88
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	2	2.85
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	2	2.85
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	2	2.85
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	8	2.82
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	14	2.8
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	14	2.8
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	14	2.8
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	6	2.79
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	14	2.76
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	12	2.75
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	12	2.75
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	12	2.75
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	7	2.75
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	2	2.73
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	2	2.73
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	2	2.73
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	2	2.73
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	2	2.73
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	15	2.73
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	6	2.72
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	6	2.72
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	11	2.72
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	2	2.71
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	2	2.71
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	4	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	12	2.69
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	14	2.67
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	14	2.67
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	14	2.67
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	8	2.65
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	8	2.65
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	8	2.65
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	20	2.65
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	20	2.65
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	20	2.65
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	8	2.65
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	1	2.64
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	2	2.61
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	3	2.6
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	17	2.6
(1,354)	1:270:A:LEU:HA	1:274:A:PHE:HD1	6	2.59
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	13	2.57
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	5	2.56
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	18	2.55
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	12	2.54
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	12	2.54
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	12	2.54
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	2	2.53
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	2	2.53
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	2	2.53
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	18	2.52
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	18	2.52
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	18	2.52
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	18	2.52
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	18	2.52
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	18	2.52
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	15	2.51
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	15	2.51
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	15	2.51
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	13	2.51
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	13	2.51
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	13	2.51
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	4	2.46
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	5	2.45
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	9	2.45
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	15	2.42
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	15	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	15	2.42
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	15	2.39
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	15	2.39
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	15	2.39
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	9	2.38
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	18	2.36
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	16	2.34
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	16	2.34
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	16	2.34
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	6	2.34
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	6	2.34
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	6	2.34
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	6	2.34
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	6	2.34
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	6	2.34
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	19	2.27
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	19	2.27
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	19	2.27
(1,359)	1:273:A:THR:H	1:274:A:PHE:HD1	15	2.25
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	2	2.17
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	2	2.17
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	2	2.17
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	13	2.17
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	13	2.16
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	13	2.16
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	13	2.16
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	12	2.01
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	15	1.98
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	15	1.98
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	15	1.98
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	15	1.98
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	15	1.98
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	15	1.98
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	20	1.97
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	20	1.97
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	20	1.97
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	1	1.94
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	1	1.94
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	18	1.91
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	18	1.91
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	18	1.91
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	18	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	18	1.91
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	18	1.91
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	7	1.9
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	20	1.87
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	20	1.87
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	20	1.87
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	11	1.86
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	11	1.86
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	11	1.86
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	4	1.85
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	4	1.85
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	4	1.85
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	7	1.81
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	7	1.81
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	7	1.81
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	7	1.81
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	7	1.81
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	7	1.81
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	18	1.81
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	1	1.8
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	1	1.8
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	1	1.8
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	16	1.79
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	16	1.79
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	16	1.79
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	11	1.79
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	11	1.79
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	11	1.79
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	11	1.78
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	11	1.78
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	11	1.78
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	11	1.78
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	11	1.78
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	11	1.78
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	4	1.75
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	4	1.75
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	4	1.75
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	19	1.71
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	17	1.7
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	17	1.7
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	17	1.7
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	17	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	17	1.7
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	17	1.7
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	1	1.69
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	1	1.69
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	1	1.69
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	6	1.64
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	6	1.64
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	6	1.64
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	20	1.64
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	20	1.64
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	20	1.64
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	13	1.64
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	9	1.62
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	9	1.62
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	9	1.62
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	9	1.62
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	9	1.62
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	9	1.62
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	4	1.61
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	4	1.61
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	13	1.6
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	13	1.6
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	13	1.6
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	2	1.6
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	14	1.59
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	11	1.58
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	11	1.58
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	11	1.58
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	6	1.58
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	6	1.58
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	6	1.58
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	6	1.58
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	6	1.58
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	6	1.58
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	13	1.56
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	13	1.56
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	8	1.55
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	3	1.53
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	12	1.53
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	18	1.53
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	20	1.52
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	20	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	1	1.52
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	17	1.52
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	4	1.51
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	16	1.5
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	16	1.5
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	16	1.5
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	15	1.5
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	15	1.5
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	15	1.5
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	11	1.48
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	11	1.48
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	11	1.48
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	12	1.47
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	12	1.47
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	6	1.46
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	6	1.46
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	6	1.46
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	6	1.45
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	12	1.43
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	11	1.43
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	7	1.41
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	3	1.4
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	18	1.4
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	20	1.38
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	20	1.38
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	20	1.38
(1,926)	1:323:A:ILE:HG21	1:324:A:TYR:HD1	5	1.38
(1,926)	1:323:A:ILE:HG22	1:324:A:TYR:HD1	5	1.38
(1,926)	1:323:A:ILE:HG23	1:324:A:TYR:HD1	5	1.38
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	17	1.36
(1,362)	1:274:A:PHE:H	1:274:A:PHE:HD1	15	1.35
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	6	1.33
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	6	1.33
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	15	1.33
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	15	1.33
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	15	1.33
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	15	1.33
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	15	1.33
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	15	1.33
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	8	1.32
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	8	1.32
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	8	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	9	1.3
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	9	1.3
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	9	1.3
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD11	8	1.3
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD12	8	1.3
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD13	8	1.3
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	14	1.29
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	13	1.27
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	2	1.24
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	8	1.2
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	8	1.2
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	8	1.2
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	8	1.2
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	19	1.19
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	19	1.19
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	19	1.19
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	5	1.18
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	5	1.18
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	5	1.18
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	5	1.18
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	5	1.18
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	5	1.18
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	4	1.18
(1,1181)	1:346:A:PRO:HA	1:349:A:ALA:HB1	15	1.17
(1,1181)	1:346:A:PRO:HA	1:349:A:ALA:HB2	15	1.17
(1,1181)	1:346:A:PRO:HA	1:349:A:ALA:HB3	15	1.17
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	4	1.16
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	4	1.16
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	4	1.16
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	6	1.16
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	12	1.13
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	20	1.12
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	20	1.12
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	20	1.12
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	1	1.12
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	8	1.11
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	8	1.11
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	3	1.11
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	3	1.11
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	3	1.11
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	15	1.1
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	15	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	7	1.09
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	9	1.09
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	9	1.09
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	9	1.09
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	9	1.09
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	9	1.09
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	9	1.09
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	12	1.09
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	14	1.07
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	14	1.07
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	14	1.07
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	4	1.07
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	4	1.07
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	4	1.07
(1,1417)	1:333:A:ILE:HD11	1:392:A:TYR:HD1	14	1.07
(1,1417)	1:333:A:ILE:HD12	1:392:A:TYR:HD1	14	1.07
(1,1417)	1:333:A:ILE:HD13	1:392:A:TYR:HD1	14	1.07
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	13	1.05
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	15	1.01
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	18	1.01
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	20	1.0
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	20	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	4	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	6	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	7	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	9	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	17	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	19	1.0
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	2	0.99
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	20	0.99
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	11	0.99
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	3	0.98
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	11	0.98
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	14	0.98
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	16	0.98
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	8	0.98
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	8	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	8	0.98
(1,1684)	1:437:A:ASP:HA	1:438:A:ASP:H	5	0.97
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	1	0.97
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	13	0.97
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	8	0.96
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	7	0.93
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	3	0.92
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	3	0.92
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	3	0.92
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	5	0.87
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	5	0.87
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	17	0.87
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	17	0.87
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	17	0.87
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	17	0.87
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	17	0.87
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	17	0.87
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	9	0.84
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	9	0.84
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	9	0.84
(1,364)	1:274:A:PHE:H	1:274:A:PHE:HE1	15	0.84
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	12	0.81
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	12	0.81
(1,538)	1:288:A:THR:HA	1:290:A:GLU:H	6	0.8
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	13	0.8
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	13	0.8
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	13	0.8
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	13	0.8
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	13	0.8
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	13	0.8
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	9	0.79
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	9	0.79
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	9	0.79
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	3	0.79
(1,424)	1:277:A:LEU:HG	1:279:A:PHE:HD1	14	0.79
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	13	0.78
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	13	0.78
(1,480)	1:238:A:ILE:HD11	1:282:A:LYS:H	3	0.77
(1,480)	1:238:A:ILE:HD12	1:282:A:LYS:H	3	0.77
(1,480)	1:238:A:ILE:HD13	1:282:A:LYS:H	3	0.77
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	5	0.77
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	5	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	5	0.77
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	5	0.77
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	5	0.77
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	5	0.77
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	18	0.77
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	18	0.77
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	18	0.77
(1,1190)	1:348:A:LEU:HA	1:351:A:LYS:H	11	0.75
(1,439)	1:235:A:TYR:HD1	1:280:A:GLU:HB2	3	0.75
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	18	0.75
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	18	0.75
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	18	0.75
(1,162)	1:247:A:ALA:HA	1:249:A:GLU:H	4	0.75
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	13	0.74
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	13	0.74
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	13	0.74
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	11	0.74
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	11	0.74
(1,1148)	1:341:A:THR:H	1:345:A:CYS:H	15	0.73
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	15	0.72
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	15	0.72
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	15	0.72
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	20	0.72
(1,1771)	1:443:A:LEU:H	1:444:A:THR:H	3	0.71
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	14	0.71
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	14	0.71
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	14	0.71
(1,314)	1:267:A:ALA:HA	1:270:A:LEU:HG	12	0.71
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	1	0.71
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	19	0.7
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	1	0.7
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	1	0.7
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	15	0.7
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	15	0.7
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	9	0.7
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	9	0.7
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	9	0.7
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	14	0.7
(1,1149)	1:341:A:THR:HB	1:345:A:CYS:H	15	0.69
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	11	0.69
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	11	0.69
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:325:A:GLY:H	1:329:A:GLN:H	20	0.68
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	14	0.67
(1,132)	1:245:A:ALA:HB1	1:246:A:LYS:H	7	0.67
(1,132)	1:245:A:ALA:HB2	1:246:A:LYS:H	7	0.67
(1,132)	1:245:A:ALA:HB3	1:246:A:LYS:H	7	0.67
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	4	0.65
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	4	0.65
(1,1375)	1:380:A:TYR:HD1	1:381:A:LEU:HA	10	0.65
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	10	0.65
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	10	0.65
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	1	0.65
(1,433)	1:235:A:TYR:HA	1:280:A:GLU:H	3	0.64
(1,499)	1:239:A:ILE:HG13	1:284:A:HIS:H	6	0.63
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	2	0.63
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	2	0.63
(1,152)	1:246:A:LYS:HA	1:248:A:ARG:H	14	0.63
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	13	0.62
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	13	0.62
(1,1160)	1:342:A:GLY:HA3	1:346:A:PRO:HA	15	0.62
(1,1110)	1:341:A:THR:HB	1:343:A:LEU:HG	17	0.62
(1,426)	1:277:A:LEU:HD11	1:279:A:PHE:HD1	13	0.62
(1,426)	1:277:A:LEU:HD12	1:279:A:PHE:HD1	13	0.62
(1,426)	1:277:A:LEU:HD13	1:279:A:PHE:HD1	13	0.62
(1,426)	1:277:A:LEU:HD21	1:279:A:PHE:HD1	13	0.62
(1,426)	1:277:A:LEU:HD22	1:279:A:PHE:HD1	13	0.62
(1,426)	1:277:A:LEU:HD23	1:279:A:PHE:HD1	13	0.62
(1,1285)	1:369:A:ILE:HA	1:369:A:ILE:HD11	20	0.61
(1,1285)	1:369:A:ILE:HA	1:369:A:ILE:HD12	20	0.61
(1,1285)	1:369:A:ILE:HA	1:369:A:ILE:HD13	20	0.61
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	16	0.61
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD11	2	0.61
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD12	2	0.61
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD13	2	0.61
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB2	4	0.61
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB3	4	0.61
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	14	0.6
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	14	0.6
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	5	0.59
(1,319)	1:269:A:ALA:HB1	1:270:A:LEU:HG	12	0.59
(1,319)	1:269:A:ALA:HB2	1:270:A:LEU:HG	12	0.59
(1,319)	1:269:A:ALA:HB3	1:270:A:LEU:HG	12	0.59
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	11	0.59
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	11	0.59
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	11	0.59
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	11	0.59
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	11	0.59
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB2	19	0.59
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB3	19	0.59
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	15	0.58
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	15	0.58
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	2	0.58
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	2	0.58
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	12	0.58
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	12	0.58
(1,553)	1:288:A:THR:H	1:291:A:GLN:HG2	6	0.58
(1,553)	1:288:A:THR:H	1:291:A:GLN:HG3	6	0.58
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	6	0.58
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	6	0.58
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	6	0.58
(1,162)	1:247:A:ALA:HA	1:249:A:GLU:H	19	0.58
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	19	0.57
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	19	0.57
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	16	0.57
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	16	0.57
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	16	0.57
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	16	0.57
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	16	0.57
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	16	0.57
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG2	6	0.57
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG3	6	0.57
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG2	6	0.57
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG3	6	0.57
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	10	0.57
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	4	0.57
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	5	0.56
(1,1954)	1:226:A:TYR:H	1:475:A:VAL:H	5	0.56
(1,1204)	1:311:A:ILE:HD11	1:354:A:VAL:HB	11	0.56
(1,1204)	1:311:A:ILE:HD12	1:354:A:VAL:HB	11	0.56
(1,1204)	1:311:A:ILE:HD13	1:354:A:VAL:HB	11	0.56
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	1	0.55
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	1	0.55
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	1	0.55
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD11	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD12	12	0.55
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD13	12	0.55
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD21	12	0.55
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD22	12	0.55
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD23	12	0.55
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	5	0.55
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	5	0.55
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	5	0.55
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	5	0.55
(1,1985)	1:310:A:PHE:H	1:476:A:PHE:HZ	12	0.54
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	6	0.54
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	6	0.54
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	19	0.54
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	19	0.54
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	19	0.54
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	17	0.54
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	19	0.54
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	19	0.54
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	5	0.53
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	5	0.53
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	19	0.53
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	19	0.53
(1,1149)	1:341:A:THR:HB	1:345:A:CYS:H	11	0.53
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	3	0.53
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	3	0.53
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	13	0.53
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	13	0.53
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	13	0.53
(1,71)	1:232:A:PRO:HA	1:234:A:GLY:H	12	0.53
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB2	1	0.53
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB3	1	0.53
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG11	7	0.52
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG12	7	0.52
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG13	7	0.52
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG21	7	0.52
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG22	7	0.52
(1,1793)	1:428:A:SER:HB2	1:446:A:VAL:HG23	7	0.52
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG11	7	0.52
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG12	7	0.52
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG13	7	0.52
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG21	7	0.52
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG22	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1793)	1:428:A:SER:HB3	1:446:A:VAL:HG23	7	0.52
(1,1018)	1:333:A:ILE:HG21	1:335:A:GLU:H	16	0.52
(1,1018)	1:333:A:ILE:HG22	1:335:A:GLU:H	16	0.52
(1,1018)	1:333:A:ILE:HG23	1:335:A:GLU:H	16	0.52
(1,551)	1:288:A:THR:HG21	1:291:A:GLN:H	6	0.52
(1,551)	1:288:A:THR:HG22	1:291:A:GLN:H	6	0.52
(1,551)	1:288:A:THR:HG23	1:291:A:GLN:H	6	0.52
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	15	0.52
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	15	0.52
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	15	0.52
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	15	0.52
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	19	0.52
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	19	0.52
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	19	0.52
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB2	3	0.52
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB3	3	0.52
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	18	0.51
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	18	0.51
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD3	16	0.51
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD3	16	0.51
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD3	16	0.51
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD3	16	0.51
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD3	16	0.51
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD2	16	0.51
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD3	16	0.51
(1,1891)	1:225:A:VAL:HA	1:473:A:LYS:HG2	20	0.51
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	8	0.51
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	7	0.51
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	11	0.51
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	11	0.51
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	18	0.51
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	18	0.51
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	18	0.51
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	16	0.51
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	7	0.51
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	2	0.51
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	11	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	11	0.51
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	11	0.51
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	14	0.51
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	14	0.51
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	14	0.51
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	4	0.51
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	4	0.51
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	4	0.51
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	20	0.51
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	20	0.51
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB2	2	0.51
(1,64)	1:231:A:LYS:HA	1:232:A:PRO:HB3	2	0.51
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE3	17	0.5
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE3	17	0.5
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE3	17	0.5
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE3	17	0.5
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE3	17	0.5
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE2	17	0.5
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE3	17	0.5
(1,1465)	1:355:A:PHE:H	1:400:A:LEU:HB2	6	0.5
(1,1465)	1:355:A:PHE:H	1:400:A:LEU:HB3	6	0.5
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	11	0.5
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	11	0.5
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	11	0.5
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD11	17	0.5
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD12	17	0.5
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD13	17	0.5
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	6	0.5
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	6	0.5
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	6	0.5
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	13	0.5
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	13	0.5
(1,1379)	1:381:A:LEU:HA	1:381:A:LEU:HG	6	0.49
(1,1172)	1:348:A:LEU:H	1:348:A:LEU:HG	8	0.49
(1,988)	1:329:A:GLN:HA	1:330:A:GLU:H	11	0.49
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD11	2	0.49
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD12	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD13	2	0.49
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	3	0.49
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	16	0.49
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	16	0.49
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	16	0.49
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	10	0.48
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	10	0.48
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	12	0.48
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	12	0.48
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	15	0.48
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	15	0.48
(1,1891)	1:225:A:VAL:HA	1:473:A:LYS:HG2	5	0.48
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	5	0.48
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	11	0.48
(1,1379)	1:381:A:LEU:HA	1:381:A:LEU:HG	2	0.48
(1,968)	1:324:A:TYR:HA	1:329:A:GLN:H	9	0.48
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	10	0.48
(1,604)	1:292:A:ILE:HG21	1:293:A:TYR:HE1	6	0.48
(1,604)	1:292:A:ILE:HG22	1:293:A:TYR:HE1	6	0.48
(1,604)	1:292:A:ILE:HG23	1:293:A:TYR:HE1	6	0.48
(1,289)	1:265:A:LEU:HB3	1:266:A:ASP:H	19	0.48
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	3	0.48
(1,17)	1:225:A:VAL:HA	1:226:A:TYR:H	5	0.48
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	3	0.47
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	3	0.47
(1,1891)	1:225:A:VAL:HA	1:473:A:LYS:HG2	17	0.47
(1,1685)	1:438:A:ASP:H	1:438:A:ASP:HB2	5	0.47
(1,1685)	1:438:A:ASP:H	1:438:A:ASP:HB3	5	0.47
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB2	16	0.47
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB3	16	0.47
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB2	16	0.47
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB3	16	0.47
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	5	0.47
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	5	0.47
(1,17)	1:225:A:VAL:HA	1:226:A:TYR:H	13	0.47
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	14	0.46
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	14	0.46
(1,1726)	1:429:A:LEU:H	1:442:A:ILE:HG21	7	0.46
(1,1726)	1:429:A:LEU:H	1:442:A:ILE:HG22	7	0.46
(1,1726)	1:429:A:LEU:H	1:442:A:ILE:HG23	7	0.46
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	15	0.46
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	15	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	15	0.46
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	15	0.46
(1,1202)	1:311:A:ILE:HG21	1:354:A:VAL:HB	11	0.46
(1,1202)	1:311:A:ILE:HG22	1:354:A:VAL:HB	11	0.46
(1,1202)	1:311:A:ILE:HG23	1:354:A:VAL:HB	11	0.46
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB1	11	0.46
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB2	11	0.46
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB3	11	0.46
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB1	11	0.46
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB2	11	0.46
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB3	11	0.46
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	18	0.46
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	18	0.46
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	18	0.46
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	20	0.46
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD11	8	0.46
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD12	8	0.46
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD13	8	0.46
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	8	0.46
(1,307)	1:267:A:ALA:HB1	1:268:A:GLY:H	12	0.46
(1,307)	1:267:A:ALA:HB2	1:268:A:GLY:H	12	0.46
(1,307)	1:267:A:ALA:HB3	1:268:A:GLY:H	12	0.46
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	1	0.46
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	15	0.46
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	15	0.46
(1,123)	1:243:A:ASN:HA	1:244:A:PHE:H	6	0.46
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	11	0.45
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	11	0.45
(1,1536)	1:422:A:ILE:HB	1:423:A:GLN:HA	8	0.45
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	19	0.45
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	19	0.45
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	16	0.45
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	16	0.45
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	16	0.45
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	3	0.45
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG2	5	0.45
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG3	5	0.45
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG2	5	0.45
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG3	5	0.45
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	16	0.44
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	16	0.44
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	20	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	20	0.44
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB3	10	0.44
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB3	10	0.44
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB3	10	0.44
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB3	10	0.44
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB3	10	0.44
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB2	10	0.44
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB3	10	0.44
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	13	0.44
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	13	0.44
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	13	0.44
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	8	0.44
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	8	0.44
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	8	0.44
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	19	0.44
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	19	0.44
(1,1338)	1:373:A:THR:HB	1:380:A:TYR:HA	2	0.44
(1,1096)	1:339:A:GLN:HA	1:341:A:THR:H	11	0.44
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	16	0.44
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	16	0.44
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	16	0.44
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	13	0.44
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	13	0.44
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	13	0.44
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	5	0.44
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	5	0.44
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	17	0.43
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	17	0.43
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	8	0.43
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	8	0.43
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	8	0.43
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	8	0.43
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	10	0.43
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	10	0.43
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	10	0.43
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	10	0.43
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	7	0.43
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	7	0.43
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	4	0.43
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	4	0.43
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	4	0.43
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	4	0.43
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	4	0.43
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	4	0.43
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	4	0.43
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	4	0.43
(1,1233)	1:312:A:CYS:H	1:356:A:PHE:H	18	0.43
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	9	0.43
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	5	0.43
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	5	0.43
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	5	0.43
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	11	0.43
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	9	0.43
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	9	0.43
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	9	0.43
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	17	0.43
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	17	0.43
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	17	0.43
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	4	0.43
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	4	0.43
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	4	0.43
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	18	0.43
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	9	0.42
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	9	0.42
(1,1891)	1:225:A:VAL:HA	1:473:A:LYS:HG2	16	0.42
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB2	17	0.42
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB3	17	0.42
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB2	17	0.42
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB3	17	0.42
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	9	0.42
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	9	0.42
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	9	0.42
(1,1459)	1:353:A:LYS:H	1:400:A:LEU:H	6	0.42
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	10	0.42
(1,1172)	1:348:A:LEU:H	1:348:A:LEU:HG	13	0.42
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	4	0.42
(1,968)	1:324:A:TYR:HA	1:329:A:GLN:H	13	0.42
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA2	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA3	9	0.42
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA2	9	0.42
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA3	9	0.42
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG21	3	0.42
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG22	3	0.42
(1,904)	1:322:A:ILE:H	1:322:A:ILE:HG23	3	0.42
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	19	0.42
(1,227)	1:253:A:LYS:HE2	1:254:A:LEU:HG	6	0.42
(1,227)	1:253:A:LYS:HE3	1:254:A:LEU:HG	6	0.42
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	14	0.42
(1,131)	1:245:A:ALA:H	1:246:A:LYS:H	7	0.42
(1,17)	1:225:A:VAL:HA	1:226:A:TYR:H	17	0.42
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	1	0.41
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	1	0.41
(1,1902)	1:226:A:TYR:H	1:473:A:LYS:HG2	13	0.41
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	2	0.41
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	15	0.41
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	15	0.41
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	15	0.41
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	15	0.41
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	15	0.41
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	15	0.41
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	19	0.41
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	19	0.41
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	19	0.41
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	9	0.41
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	9	0.41
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	20	0.41
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	20	0.41
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	20	0.41
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	20	0.41
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	20	0.41
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	20	0.41
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	2	0.41
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	11	0.41
(1,1153)	1:343:A:LEU:H	1:345:A:CYS:H	15	0.41
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	19	0.41
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	2	0.41
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	2	0.41
(1,944)	1:247:A:ALA:H	1:327:A:ASP:H	14	0.41
(1,940)	1:246:A:LYS:HB2	1:327:A:ASP:HA	7	0.41
(1,940)	1:246:A:LYS:HB3	1:327:A:ASP:HA	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	15	0.41
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	15	0.41
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	9	0.41
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	18	0.41
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD11	14	0.41
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD12	14	0.41
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD13	14	0.41
(1,231)	1:254:A:LEU:H	1:254:A:LEU:HG	18	0.41
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB2	4	0.41
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB3	4	0.41
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG2	18	0.4
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG3	18	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD11	15	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD12	15	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD13	15	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD21	15	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD22	15	0.4
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD23	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD11	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD12	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD13	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD21	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD22	15	0.4
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD23	15	0.4
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	6	0.4
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	6	0.4
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	6	0.4
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	6	0.4
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	19	0.4
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	5	0.4
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	9	0.4
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	14	0.4
(1,915)	1:322:A:ILE:HG12	1:323:A:ILE:H	5	0.4
(1,915)	1:322:A:ILE:HG13	1:323:A:ILE:H	5	0.4
(1,795)	1:307:A:MET:HE1	1:309:A:CYS:H	15	0.4
(1,795)	1:307:A:MET:HE2	1:309:A:CYS:H	15	0.4
(1,795)	1:307:A:MET:HE3	1:309:A:CYS:H	15	0.4
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	14	0.4
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	14	0.4
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	14	0.4
(1,448)	1:238:A:ILE:HD11	1:281:A:ILE:HA	3	0.4
(1,448)	1:238:A:ILE:HD12	1:281:A:ILE:HA	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:238:A:ILE:HD13	1:281:A:ILE:HA	3	0.4
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	4	0.4
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	19	0.4
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	19	0.4
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	19	0.4
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	18	0.4
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	18	0.4
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	18	0.4
(1,124)	1:243:A:ASN:HB2	1:245:A:ALA:H	18	0.4
(1,124)	1:243:A:ASN:HB3	1:245:A:ALA:H	18	0.4
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD11	10	0.39
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD12	10	0.39
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD13	10	0.39
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	7	0.39
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	7	0.39
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	7	0.39
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	7	0.39
(1,1375)	1:380:A:TYR:HD1	1:381:A:LEU:HA	5	0.39
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	19	0.39
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	19	0.39
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	19	0.39
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	19	0.39
(1,1356)	1:373:A:THR:HB	1:381:A:LEU:HG	3	0.39
(1,1316)	1:373:A:THR:HA	1:374:A:ASP:HA	17	0.39
(1,969)	1:325:A:GLY:H	1:329:A:GLN:H	16	0.39
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	20	0.39
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	20	0.39
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	8	0.39
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	8	0.39
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	8	0.39
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD11	4	0.39
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD12	4	0.39
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD13	4	0.39
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG2	4	0.39
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG2	4	0.39
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG2	4	0.39
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG3	4	0.39
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG3	4	0.39
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG3	4	0.39
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	19	0.39
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	16	0.39
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	16	0.39
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	2	0.39
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	2	0.39
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	2	0.39
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	2	0.39
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	2	0.39
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	2	0.39
(1,163)	1:248:A:ARG:HG2	1:249:A:GLU:H	4	0.39
(1,163)	1:248:A:ARG:HG3	1:249:A:GLU:H	4	0.39
(1,1984)	1:310:A:PHE:H	1:476:A:PHE:HE1	11	0.38
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	4	0.38
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	4	0.38
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	8	0.38
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	8	0.38
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	10	0.38
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	10	0.38
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	10	0.38
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	10	0.38
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	10	0.38
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	10	0.38
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	8	0.38
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	8	0.38
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	8	0.38
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	8	0.38
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	12	0.38
(1,1340)	1:376:A:GLU:HA	1:380:A:TYR:HA	12	0.38
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG2	14	0.38
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG3	14	0.38
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG2	14	0.38
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG3	14	0.38
(1,1315)	1:373:A:THR:HB	1:374:A:ASP:HA	10	0.38
(1,933)	1:324:A:TYR:HB3	1:325:A:GLY:H	3	0.38
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	11	0.38
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	8	0.38
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	8	0.38
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	8	0.38
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	8	0.38
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	8	0.38
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	8	0.38
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	2	0.38
(1,171)	1:247:A:ALA:HA	1:250:A:LYS:HB2	11	0.38
(1,171)	1:247:A:ALA:HA	1:250:A:LYS:HB3	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:243:A:ASN:HA	1:244:A:PHE:H	13	0.38
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	3	0.37
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	5	0.37
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD11	7	0.37
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD12	7	0.37
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD13	7	0.37
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	7	0.37
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	7	0.37
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	20	0.37
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	20	0.37
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	20	0.37
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	11	0.37
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	11	0.37
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	11	0.37
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	6	0.37
(1,1126)	1:341:A:THR:H	1:344:A:LYS:H	15	0.37
(1,1019)	1:333:A:ILE:H	1:335:A:GLU:H	11	0.37
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB2	18	0.37
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB3	18	0.37
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	18	0.37
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG2	2	0.37
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG3	2	0.37
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	13	0.37
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	13	0.37
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	13	0.37
(1,318)	1:269:A:ALA:HB1	1:270:A:LEU:H	12	0.37
(1,318)	1:269:A:ALA:HB2	1:270:A:LEU:H	12	0.37
(1,318)	1:269:A:ALA:HB3	1:270:A:LEU:H	12	0.37
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	17	0.37
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	17	0.37
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	17	0.37
(1,243)	1:254:A:LEU:HA	1:256:A:SER:H	13	0.37
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	2	0.37
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	6	0.37
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	6	0.37
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	15	0.37
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	15	0.37
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	11	0.37
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	11	0.37
(1,2016)	1:477:A:PRO:HB2	1:478:A:SER:HB2	11	0.36
(1,2016)	1:477:A:PRO:HB2	1:478:A:SER:HB3	11	0.36
(1,1771)	1:443:A:LEU:H	1:444:A:THR:H	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	8	0.36
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	8	0.36
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	8	0.36
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	16	0.36
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	16	0.36
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	16	0.36
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	16	0.36
(1,1110)	1:341:A:THR:HB	1:343:A:LEU:HG	20	0.36
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	13	0.36
(1,940)	1:246:A:LYS:HB2	1:327:A:ASP:HA	14	0.36
(1,940)	1:246:A:LYS:HB3	1:327:A:ASP:HA	14	0.36
(1,913)	1:322:A:ILE:HG21	1:323:A:ILE:H	15	0.36
(1,913)	1:322:A:ILE:HG22	1:323:A:ILE:H	15	0.36
(1,913)	1:322:A:ILE:HG23	1:323:A:ILE:H	15	0.36
(1,896)	1:319:A:ASP:HB2	1:322:A:ILE:HG12	11	0.36
(1,896)	1:319:A:ASP:HB2	1:322:A:ILE:HG13	11	0.36
(1,896)	1:319:A:ASP:HB3	1:322:A:ILE:HG12	11	0.36
(1,896)	1:319:A:ASP:HB3	1:322:A:ILE:HG13	11	0.36
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	2	0.36
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	2	0.36
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB2	10	0.36
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB3	10	0.36
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	5	0.36
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	12	0.36
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	12	0.36
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	12	0.36
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	12	0.36
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	12	0.36
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	12	0.36
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	12	0.36
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	12	0.36
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	12	0.36
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG2	14	0.36
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG3	14	0.36
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB2	19	0.36
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB3	19	0.36
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB2	14	0.36
(1,164)	1:248:A:ARG:H	1:249:A:GLU:HB3	14	0.36
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	9	0.36
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	9	0.36
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	9	0.36
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	9	0.36
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	9	0.36
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	4	0.35
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	4	0.35
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	14	0.35
(1,1462)	1:354:A:VAL:HG11	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG11	1:400:A:LEU:HB3	6	0.35
(1,1462)	1:354:A:VAL:HG12	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG12	1:400:A:LEU:HB3	6	0.35
(1,1462)	1:354:A:VAL:HG13	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG13	1:400:A:LEU:HB3	6	0.35
(1,1462)	1:354:A:VAL:HG21	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG21	1:400:A:LEU:HB3	6	0.35
(1,1462)	1:354:A:VAL:HG22	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG22	1:400:A:LEU:HB3	6	0.35
(1,1462)	1:354:A:VAL:HG23	1:400:A:LEU:HB2	6	0.35
(1,1462)	1:354:A:VAL:HG23	1:400:A:LEU:HB3	6	0.35
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	9	0.35
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	9	0.35
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	9	0.35
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	2	0.35
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	2	0.35
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	2	0.35
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	2	0.35
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	2	0.35
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	2	0.35
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	17	0.35
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	17	0.35
(1,1192)	1:349:A:ALA:HA	1:351:A:LYS:H	15	0.35
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	17	0.35
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	15	0.35
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG21	16	0.35
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG22	16	0.35
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG23	16	0.35
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	13	0.35
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	13	0.35
(1,949)	1:326:A:THR:H	1:327:A:ASP:H	19	0.35
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG12	6	0.35
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG13	6	0.35
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	17	0.35
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	17	0.35
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	12	0.35
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	12	0.35
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	11	0.35
(1,432)	1:234:A:GLY:H	1:280:A:GLU:H	8	0.35
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	12	0.35
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	15	0.35
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	15	0.35
(1,2012)	1:277:A:LEU:HD11	1:478:A:SER:HA	3	0.34
(1,2012)	1:277:A:LEU:HD12	1:478:A:SER:HA	3	0.34
(1,2012)	1:277:A:LEU:HD13	1:478:A:SER:HA	3	0.34
(1,2012)	1:277:A:LEU:HD21	1:478:A:SER:HA	3	0.34
(1,2012)	1:277:A:LEU:HD22	1:478:A:SER:HA	3	0.34
(1,2012)	1:277:A:LEU:HD23	1:478:A:SER:HA	3	0.34
(1,1990)	1:438:A:ASP:HA	1:476:A:PHE:H	17	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD11	15	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD12	15	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD13	15	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD21	15	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD22	15	0.34
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD23	15	0.34
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	5	0.34
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	5	0.34
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	5	0.34
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	10	0.34
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	10	0.34
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	16	0.34
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	16	0.34
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	16	0.34
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	16	0.34
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	16	0.34
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	16	0.34
(1,1022)	1:334:A:TYR:HB2	1:335:A:GLU:H	3	0.34
(1,903)	1:322:A:ILE:H	1:322:A:ILE:HG13	6	0.34
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	6	0.34
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	6	0.34
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	20	0.34
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	20	0.34
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	14	0.34
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	17	0.34
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	9	0.34
(1,387)	1:273:A:THR:HA	1:276:A:GLU:H	8	0.34
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	1	0.34
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	1	0.34
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	17	0.34
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	17	0.34
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	17	0.34
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	11	0.34
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	11	0.34
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	11	0.34
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	5	0.34
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB2	14	0.34
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB3	14	0.34
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	3	0.34
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	3	0.34
(1,139)	1:246:A:LYS:H	1:246:A:LYS:HB2	7	0.34
(1,139)	1:246:A:LYS:H	1:246:A:LYS:HB3	7	0.34
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE2	9	0.34
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE3	9	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	5	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	5	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	5	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	5	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	5	0.34
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	5	0.34
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	5	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	4	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	4	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	4	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	4	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	4	0.34
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	4	0.34
(1,1918)	1:228:A:MET:HE1	1:474:A:LEU:HG	17	0.33
(1,1918)	1:228:A:MET:HE2	1:474:A:LEU:HG	17	0.33
(1,1918)	1:228:A:MET:HE3	1:474:A:LEU:HG	17	0.33
(1,1835)	1:398:A:ASP:H	1:470:A:LEU:HG	11	0.33
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD11	12	0.33
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD12	12	0.33
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD13	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD21	12	0.33
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD22	12	0.33
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD23	12	0.33
(1,1536)	1:422:A:ILE:HB	1:423:A:GLN:HA	1	0.33
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	2	0.33
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	2	0.33
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	2	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG21	7	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG22	7	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG23	7	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG21	11	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG22	11	0.33
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG23	11	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD11	5	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD12	5	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD13	5	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD21	5	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD22	5	0.33
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD23	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD11	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD12	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD13	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD21	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD22	5	0.33
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD23	5	0.33
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB2	10	0.33
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB3	10	0.33
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB2	10	0.33
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB3	10	0.33
(1,1189)	1:349:A:ALA:HB1	1:350:A:GLY:H	15	0.33
(1,1189)	1:349:A:ALA:HB2	1:350:A:GLY:H	15	0.33
(1,1189)	1:349:A:ALA:HB3	1:350:A:GLY:H	15	0.33
(1,1093)	1:339:A:GLN:H	1:340:A:PHE:H	11	0.33
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	7	0.33
(1,1007)	1:333:A:ILE:HB	1:334:A:TYR:H	16	0.33
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	14	0.33
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	14	0.33
(1,925)	1:323:A:ILE:HB	1:324:A:TYR:H	15	0.33
(1,865)	1:239:A:ILE:HG21	1:316:A:SER:H	5	0.33
(1,865)	1:239:A:ILE:HG22	1:316:A:SER:H	5	0.33
(1,865)	1:239:A:ILE:HG23	1:316:A:SER:H	5	0.33
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	4	0.33
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	13	0.33
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	16	0.33
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	16	0.33
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	16	0.33
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	16	0.33
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	16	0.33
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	16	0.33
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	16	0.33
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	16	0.33
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	16	0.33
(1,578)	1:289:A:VAL:HA	1:292:A:ILE:HD11	6	0.33
(1,578)	1:289:A:VAL:HA	1:292:A:ILE:HD12	6	0.33
(1,578)	1:289:A:VAL:HA	1:292:A:ILE:HD13	6	0.33
(1,514)	1:241:A:ASN:HA	1:286:A:ASP:H	1	0.33
(1,432)	1:234:A:GLY:H	1:280:A:GLU:H	18	0.33
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	4	0.33
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	4	0.33
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	4	0.33
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD11	13	0.33
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD12	13	0.33
(1,255)	1:255:A:HIS:HA	1:257:A:ILE:HD13	13	0.33
(1,224)	1:251:A:VAL:HG11	1:254:A:LEU:HG	18	0.33
(1,224)	1:251:A:VAL:HG12	1:254:A:LEU:HG	18	0.33
(1,224)	1:251:A:VAL:HG13	1:254:A:LEU:HG	18	0.33
(1,224)	1:251:A:VAL:HG21	1:254:A:LEU:HG	18	0.33
(1,224)	1:251:A:VAL:HG22	1:254:A:LEU:HG	18	0.33
(1,224)	1:251:A:VAL:HG23	1:254:A:LEU:HG	18	0.33
(1,214)	1:251:A:VAL:HB	1:254:A:LEU:H	5	0.33
(1,184)	1:250:A:LYS:HA	1:250:A:LYS:HG3	11	0.33
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	16	0.33
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	16	0.33
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	6	0.32
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	6	0.32
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	13	0.32
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	13	0.32
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG11	10	0.32
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG12	10	0.32
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG13	10	0.32
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	3	0.32
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	3	0.32
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	3	0.32
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	3	0.32
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	3	0.32
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG21	7	0.32
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG22	7	0.32
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG23	7	0.32
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG21	7	0.32
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG22	7	0.32
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG23	7	0.32
(1,1719)	1:439:A:ILE:HG21	1:441:A:THR:H	7	0.32
(1,1719)	1:439:A:ILE:HG22	1:441:A:THR:H	7	0.32
(1,1719)	1:439:A:ILE:HG23	1:441:A:THR:H	7	0.32
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB2	14	0.32
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB3	14	0.32
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB2	14	0.32
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB3	14	0.32
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	17	0.32
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	17	0.32
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	7	0.32
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	7	0.32
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	15	0.32
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	15	0.32
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	15	0.32
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	11	0.32
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	11	0.32
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	11	0.32
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	11	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	20	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	20	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	20	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	20	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	20	0.32
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	20	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG11	15	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG12	15	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG13	15	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG21	15	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG22	15	0.32
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG23	15	0.32
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG11	15	0.32
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG12	15	0.32
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG13	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG21	15	0.32
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG22	15	0.32
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG23	15	0.32
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	9	0.32
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	11	0.32
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	17	0.32
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	17	0.32
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	17	0.32
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG21	18	0.32
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG22	18	0.32
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG23	18	0.32
(1,933)	1:324:A:TYR:HB3	1:325:A:GLY:H	19	0.32
(1,912)	1:322:A:ILE:HB	1:323:A:ILE:H	15	0.32
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	2	0.32
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	1	0.32
(1,705)	1:298:A:ILE:HG21	1:299:A:TYR:HE1	4	0.32
(1,705)	1:298:A:ILE:HG22	1:299:A:TYR:HE1	4	0.32
(1,705)	1:298:A:ILE:HG23	1:299:A:TYR:HE1	4	0.32
(1,525)	1:241:A:ASN:HB2	1:287:A:CYS:H	13	0.32
(1,525)	1:241:A:ASN:HB3	1:287:A:CYS:H	13	0.32
(1,460)	1:275:A:GLU:HG2	1:281:A:ILE:HD11	3	0.32
(1,460)	1:275:A:GLU:HG2	1:281:A:ILE:HD12	3	0.32
(1,460)	1:275:A:GLU:HG2	1:281:A:ILE:HD13	3	0.32
(1,460)	1:275:A:GLU:HG3	1:281:A:ILE:HD11	3	0.32
(1,460)	1:275:A:GLU:HG3	1:281:A:ILE:HD12	3	0.32
(1,460)	1:275:A:GLU:HG3	1:281:A:ILE:HD13	3	0.32
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD11	10	0.32
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD12	10	0.32
(1,457)	1:274:A:PHE:HD1	1:281:A:ILE:HD13	10	0.32
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB2	4	0.32
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB3	4	0.32
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	3	0.32
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	13	0.32
(1,21)	1:225:A:VAL:HG11	1:226:A:TYR:H	16	0.32
(1,21)	1:225:A:VAL:HG12	1:226:A:TYR:H	16	0.32
(1,21)	1:225:A:VAL:HG13	1:226:A:TYR:H	16	0.32
(1,21)	1:225:A:VAL:HG21	1:226:A:TYR:H	16	0.32
(1,21)	1:225:A:VAL:HG22	1:226:A:TYR:H	16	0.32
(1,21)	1:225:A:VAL:HG23	1:226:A:TYR:H	16	0.32
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	12	0.32
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	12	0.32
(1,17)	1:225:A:VAL:HA	1:226:A:TYR:H	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	15	0.31
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	12	0.31
(1,1954)	1:226:A:TYR:H	1:475:A:VAL:H	17	0.31
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE3	5	0.31
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE3	5	0.31
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE3	5	0.31
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE3	5	0.31
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE3	5	0.31
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE2	5	0.31
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE3	5	0.31
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD11	6	0.31
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD12	6	0.31
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD13	6	0.31
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	10	0.31
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	8	0.31
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	14	0.31
(1,1347)	1:380:A:TYR:H	1:380:A:TYR:HD1	5	0.31
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	13	0.31
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB2	13	0.31
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB3	13	0.31
(1,1147)	1:341:A:THR:HG21	1:345:A:CYS:H	15	0.31
(1,1147)	1:341:A:THR:HG22	1:345:A:CYS:H	15	0.31
(1,1147)	1:341:A:THR:HG23	1:345:A:CYS:H	15	0.31
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	16	0.31
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	16	0.31
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	18	0.31
(1,925)	1:323:A:ILE:HB	1:324:A:TYR:H	19	0.31
(1,828)	1:311:A:ILE:HD11	1:312:A:CYS:H	12	0.31
(1,828)	1:311:A:ILE:HD12	1:312:A:CYS:H	12	0.31
(1,828)	1:311:A:ILE:HD13	1:312:A:CYS:H	12	0.31
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	12	0.31
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	12	0.31
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	12	0.31
(1,523)	1:239:A:ILE:HG21	1:287:A:CYS:H	18	0.31
(1,523)	1:239:A:ILE:HG22	1:287:A:CYS:H	18	0.31
(1,523)	1:239:A:ILE:HG23	1:287:A:CYS:H	18	0.31
(1,463)	1:279:A:PHE:H	1:281:A:ILE:HD11	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:279:A:PHE:H	1:281:A:ILE:HD12	8	0.31
(1,463)	1:279:A:PHE:H	1:281:A:ILE:HD13	8	0.31
(1,431)	1:279:A:PHE:H	1:279:A:PHE:HD1	7	0.31
(1,423)	1:277:A:LEU:H	1:279:A:PHE:H	4	0.31
(1,411)	1:276:A:GLU:HG3	1:278:A:HIS:H	10	0.31
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG2	8	0.31
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG3	8	0.31
(1,346)	1:271:A:THR:H	1:273:A:THR:H	10	0.31
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	14	0.31
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	17	0.31
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	17	0.31
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	17	0.31
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	8	0.31
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	9	0.31
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	9	0.31
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	9	0.31
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	4	0.31
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	19	0.31
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	19	0.31
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	19	0.31
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD2	4	0.31
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD3	4	0.31
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	3	0.3
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	7	0.3
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	7	0.3
(1,1954)	1:226:A:TYR:H	1:475:A:VAL:H	13	0.3
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	11	0.3
(1,1633)	1:430:A:ARG:HG2	1:431:A:GLU:H	10	0.3
(1,1633)	1:430:A:ARG:HG3	1:431:A:GLU:H	10	0.3
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	15	0.3
(1,1584)	1:425:A:LEU:HB2	1:428:A:SER:H	7	0.3
(1,1584)	1:425:A:LEU:HB3	1:428:A:SER:H	7	0.3
(1,1548)	1:422:A:ILE:H	1:425:A:LEU:H	17	0.3
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	11	0.3
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	11	0.3
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	11	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD11	15	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD12	15	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD13	15	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD21	15	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD22	15	0.3
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD23	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD11	15	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD12	15	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD13	15	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD21	15	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD22	15	0.3
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD23	15	0.3
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	17	0.3
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	17	0.3
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	17	0.3
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	17	0.3
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	18	0.3
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	18	0.3
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	18	0.3
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	18	0.3
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	6	0.3
(1,1063)	1:334:A:TYR:HA	1:337:A:THR:H	6	0.3
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	3	0.3
(1,942)	1:246:A:LYS:HD2	1:327:A:ASP:HB2	7	0.3
(1,942)	1:246:A:LYS:HD2	1:327:A:ASP:HB3	7	0.3
(1,942)	1:246:A:LYS:HD3	1:327:A:ASP:HB2	7	0.3
(1,942)	1:246:A:LYS:HD3	1:327:A:ASP:HB3	7	0.3
(1,935)	1:288:A:THR:HG21	1:326:A:THR:H	7	0.3
(1,935)	1:288:A:THR:HG22	1:326:A:THR:H	7	0.3
(1,935)	1:288:A:THR:HG23	1:326:A:THR:H	7	0.3
(1,915)	1:322:A:ILE:HG12	1:323:A:ILE:H	3	0.3
(1,915)	1:322:A:ILE:HG13	1:323:A:ILE:H	3	0.3
(1,915)	1:322:A:ILE:HG12	1:323:A:ILE:H	18	0.3
(1,915)	1:322:A:ILE:HG13	1:323:A:ILE:H	18	0.3
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	11	0.3
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	11	0.3
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	3	0.3
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	6	0.3
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	19	0.3
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	6	0.3
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	8	0.3
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	8	0.3
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	8	0.3
(1,514)	1:241:A:ASN:HA	1:286:A:ASP:H	9	0.3
(1,387)	1:273:A:THR:HA	1:276:A:GLU:H	2	0.3
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	14	0.3
(1,361)	1:273:A:THR:HG21	1:274:A:PHE:HD1	12	0.3
(1,361)	1:273:A:THR:HG22	1:274:A:PHE:HD1	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:273:A:THR:HG23	1:274:A:PHE:HD1	12	0.3
(1,289)	1:265:A:LEU:HB3	1:266:A:ASP:H	9	0.3
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	18	0.3
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	18	0.3
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	18	0.3
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	18	0.3
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	7	0.3
(1,203)	1:251:A:VAL:H	1:253:A:LYS:H	4	0.3
(1,162)	1:247:A:ALA:HA	1:249:A:GLU:H	14	0.3
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	4	0.29
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	2	0.29
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	2	0.29
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	14	0.29
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	14	0.29
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD3	5	0.29
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD3	5	0.29
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD3	5	0.29
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD3	5	0.29
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD3	5	0.29
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD2	5	0.29
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD3	5	0.29
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	13	0.29
(1,1795)	1:444:A:THR:HG21	1:446:A:VAL:H	2	0.29
(1,1795)	1:444:A:THR:HG22	1:446:A:VAL:H	2	0.29
(1,1795)	1:444:A:THR:HG23	1:446:A:VAL:H	2	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD11	6	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD12	6	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD13	6	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD21	6	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD22	6	0.29
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD23	6	0.29
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	7	0.29
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG2	1	0.29
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG3	1	0.29
(1,1649)	1:277:A:LEU:HD11	1:434:A:PRO:HD2	10	0.29
(1,1649)	1:277:A:LEU:HD11	1:434:A:PRO:HD3	10	0.29
(1,1649)	1:277:A:LEU:HD12	1:434:A:PRO:HD2	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:277:A:LEU:HD12	1:434:A:PRO:HD3	10	0.29
(1,1649)	1:277:A:LEU:HD13	1:434:A:PRO:HD2	10	0.29
(1,1649)	1:277:A:LEU:HD13	1:434:A:PRO:HD3	10	0.29
(1,1649)	1:277:A:LEU:HD21	1:434:A:PRO:HD2	10	0.29
(1,1649)	1:277:A:LEU:HD21	1:434:A:PRO:HD3	10	0.29
(1,1649)	1:277:A:LEU:HD22	1:434:A:PRO:HD2	10	0.29
(1,1649)	1:277:A:LEU:HD22	1:434:A:PRO:HD3	10	0.29
(1,1649)	1:277:A:LEU:HD23	1:434:A:PRO:HD2	10	0.29
(1,1649)	1:277:A:LEU:HD23	1:434:A:PRO:HD3	10	0.29
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	5	0.29
(1,1633)	1:430:A:ARG:HG2	1:431:A:GLU:H	8	0.29
(1,1633)	1:430:A:ARG:HG3	1:431:A:GLU:H	8	0.29
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	4	0.29
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	4	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD11	15	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD12	15	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD13	15	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD21	15	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD22	15	0.29
(1,1398)	1:384:A:ASP:HA	1:385:A:LEU:HD23	15	0.29
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	14	0.29
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	14	0.29
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	14	0.29
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	14	0.29
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	16	0.29
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	16	0.29
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	16	0.29
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	16	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	18	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	18	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	18	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	18	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	18	0.29
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	18	0.29
(1,1338)	1:373:A:THR:HB	1:380:A:TYR:HA	9	0.29
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	17	0.29
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	17	0.29
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	17	0.29
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	2	0.29
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	11	0.29
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	11	0.29
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG21	19	0.29
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG22	19	0.29
(1,1064)	1:334:A:TYR:HA	1:337:A:THR:HG23	19	0.29
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	5	0.29
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	5	0.29
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	11	0.29
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	11	0.29
(1,944)	1:247:A:ALA:H	1:327:A:ASP:H	13	0.29
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG21	14	0.29
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG22	14	0.29
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG23	14	0.29
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	12	0.29
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	12	0.29
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB2	12	0.29
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB3	12	0.29
(1,870)	1:317:A:HIS:HA	1:318:A:GLY:H	5	0.29
(1,859)	1:314:A:ILE:HG21	1:315:A:LEU:H	2	0.29
(1,859)	1:314:A:ILE:HG22	1:315:A:LEU:H	2	0.29
(1,859)	1:314:A:ILE:HG23	1:315:A:LEU:H	2	0.29
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	16	0.29
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	2	0.29
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	2	0.29
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	2	0.29
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	2	0.29
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	2	0.29
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	2	0.29
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	2	0.29
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	2	0.29
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	2	0.29
(1,534)	1:288:A:THR:HB	1:289:A:VAL:H	14	0.29
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	18	0.29
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	18	0.29
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	18	0.29
(1,440)	1:236:A:CYS:H	1:280:A:GLU:H	17	0.29
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	3	0.29
(1,227)	1:253:A:LYS:HE2	1:254:A:LEU:HG	18	0.29
(1,227)	1:253:A:LYS:HE3	1:254:A:LEU:HG	18	0.29
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	6	0.29
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	2	0.29
(1,1951)	1:225:A:VAL:HA	1:475:A:VAL:H	5	0.28
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	7	0.28
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	7	0.28
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	7	0.28
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	7	0.28
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	7	0.28
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	8	0.28
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	8	0.28
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	8	0.28
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	13	0.28
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	13	0.28
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	13	0.28
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	13	0.28
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	13	0.28
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	13	0.28
(1,1442)	1:396:A:GLU:HA	1:397:A:ALA:H	19	0.28
(1,1409)	1:389:A:GLN:HG2	1:390:A:THR:HA	12	0.28
(1,1409)	1:389:A:GLN:HG3	1:390:A:THR:HA	12	0.28
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG2	2	0.28
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG3	2	0.28
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG2	2	0.28
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG3	2	0.28
(1,1190)	1:348:A:LEU:HA	1:351:A:LYS:H	7	0.28
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	7	0.28
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	14	0.28
(1,990)	1:329:A:GLN:HB2	1:330:A:GLU:H	11	0.28
(1,990)	1:329:A:GLN:HB3	1:330:A:GLU:H	11	0.28
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	12	0.28
(1,800)	1:309:A:CYS:HA	1:310:A:PHE:H	12	0.28
(1,795)	1:307:A:MET:HE1	1:309:A:CYS:H	13	0.28
(1,795)	1:307:A:MET:HE2	1:309:A:CYS:H	13	0.28
(1,795)	1:307:A:MET:HE3	1:309:A:CYS:H	13	0.28
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	14	0.28
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	7	0.28
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	8	0.28
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	1	0.28
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	13	0.28
(1,465)	1:280:A:GLU:HB3	1:281:A:ILE:H	7	0.28
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	14	0.28
(1,325)	1:238:A:ILE:HD11	1:271:A:THR:HB	6	0.28
(1,325)	1:238:A:ILE:HD12	1:271:A:THR:HB	6	0.28
(1,325)	1:238:A:ILE:HD13	1:271:A:THR:HB	6	0.28
(1,291)	1:265:A:LEU:HB2	1:266:A:ASP:H	19	0.28
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	15	0.28
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	5	0.28
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	17	0.28
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	17	0.28
(1,154)	1:247:A:ALA:HB1	1:248:A:ARG:H	18	0.28
(1,154)	1:247:A:ALA:HB2	1:248:A:ARG:H	18	0.28
(1,154)	1:247:A:ALA:HB3	1:248:A:ARG:H	18	0.28
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	10	0.28
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	4	0.28
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	4	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	16	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	16	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	16	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	16	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	16	0.28
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	16	0.28
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	16	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	20	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	20	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	20	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	20	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	20	0.28
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	20	0.28
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	2	0.27
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	8	0.27
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	8	0.27
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG21	1	0.27
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG22	1	0.27
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG23	1	0.27
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	17	0.27
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB2	12	0.27
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB3	12	0.27
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB2	12	0.27
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB3	12	0.27
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB2	12	0.27
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB3	12	0.27
(1,1419)	1:333:A:ILE:HG21	1:392:A:TYR:HD1	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	1:333:A:ILE:HG22	1:392:A:TYR:HD1	14	0.27
(1,1419)	1:333:A:ILE:HG23	1:392:A:TYR:HD1	14	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	15	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	15	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	15	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	15	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	15	0.27
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	15	0.27
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	15	0.27
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	8	0.27
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	20	0.27
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	20	0.27
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	10	0.27
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	10	0.27
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	10	0.27
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	10	0.27
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	10	0.27
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	10	0.27
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	4	0.27
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	13	0.27
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	13	0.27
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	13	0.27
(1,1172)	1:348:A:LEU:H	1:348:A:LEU:HG	11	0.27
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	20	0.27
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG21	16	0.27
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG22	16	0.27
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG23	16	0.27
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG21	16	0.27
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG22	16	0.27
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG23	16	0.27
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG21	16	0.27
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG22	16	0.27
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG23	16	0.27
(1,1057)	1:296:A:LEU:HD11	1:337:A:THR:H	11	0.27
(1,1057)	1:296:A:LEU:HD12	1:337:A:THR:H	11	0.27
(1,1057)	1:296:A:LEU:HD13	1:337:A:THR:H	11	0.27
(1,1057)	1:296:A:LEU:HD21	1:337:A:THR:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:296:A:LEU:HD22	1:337:A:THR:H	11	0.27
(1,1057)	1:296:A:LEU:HD23	1:337:A:THR:H	11	0.27
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	10	0.27
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	20	0.27
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	20	0.27
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	20	0.27
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB1	2	0.27
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB2	2	0.27
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB3	2	0.27
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA2	20	0.27
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA3	20	0.27
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	9	0.27
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	9	0.27
(1,926)	1:323:A:ILE:HG21	1:324:A:TYR:HD1	15	0.27
(1,926)	1:323:A:ILE:HG22	1:324:A:TYR:HD1	15	0.27
(1,926)	1:323:A:ILE:HG23	1:324:A:TYR:HD1	15	0.27
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB2	20	0.27
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB3	20	0.27
(1,856)	1:239:A:ILE:H	1:315:A:LEU:H	8	0.27
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	8	0.27
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	8	0.27
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	8	0.27
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	10	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD11	15	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD12	15	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD13	15	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD21	15	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD22	15	0.27
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD23	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD11	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD12	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD13	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD21	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD22	15	0.27
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD23	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD11	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD12	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD13	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD21	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD22	15	0.27
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD23	15	0.27
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:289:A:VAL:H	1:292:A:ILE:HD11	6	0.27
(1,573)	1:289:A:VAL:H	1:292:A:ILE:HD12	6	0.27
(1,573)	1:289:A:VAL:H	1:292:A:ILE:HD13	6	0.27
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	2	0.27
(1,422)	1:275:A:GLU:HA	1:279:A:PHE:H	8	0.27
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	12	0.27
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	9	0.27
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	2	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD11	9	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD12	9	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD13	9	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD21	9	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD22	9	0.27
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD23	9	0.27
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	15	0.27
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG2	1	0.27
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG3	1	0.27
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG2	1	0.27
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG3	1	0.27
(1,175)	1:249:A:GLU:HB2	1:250:A:LYS:H	19	0.27
(1,175)	1:249:A:GLU:HB3	1:250:A:LYS:H	19	0.27
(1,72)	1:232:A:PRO:HB2	1:234:A:GLY:H	5	0.27
(1,72)	1:232:A:PRO:HB3	1:234:A:GLY:H	5	0.27
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	14	0.27
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	14	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	12	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	12	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	12	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	12	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	12	0.27
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	12	0.27
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	8	0.26
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	8	0.26
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	13	0.26
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	1	0.26
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	1	0.26
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD11	14	0.26
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD12	14	0.26
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD13	14	0.26
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	11	0.26
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	20	0.26
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	20	0.26
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG21	9	0.26
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG22	9	0.26
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG23	9	0.26
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG21	9	0.26
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG22	9	0.26
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG23	9	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD11	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD12	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD13	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD21	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD22	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD23	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD11	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD12	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD13	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD21	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD22	2	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD23	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD11	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD12	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD13	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD21	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD22	2	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD23	2	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD11	17	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD12	17	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD13	17	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD21	17	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD22	17	0.26
(1,1708)	1:439:A:ILE:HG21	1:440:A:LEU:HD23	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD11	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD12	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD13	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD21	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD22	17	0.26
(1,1708)	1:439:A:ILE:HG22	1:440:A:LEU:HD23	17	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD11	17	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD12	17	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD13	17	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD21	17	0.26
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD22	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:439:A:ILE:HG23	1:440:A:LEU:HD23	17	0.26
(1,1487)	1:355:A:PHE:H	1:402:A:GLY:H	11	0.26
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	4	0.26
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	4	0.26
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	4	0.26
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	4	0.26
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	18	0.26
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	18	0.26
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	18	0.26
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	18	0.26
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	18	0.26
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	18	0.26
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB2	4	0.26
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB3	4	0.26
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB2	4	0.26
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB3	4	0.26
(1,1109)	1:341:A:THR:HB	1:343:A:LEU:HB2	15	0.26
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB2	13	0.26
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB3	13	0.26
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	5	0.26
(1,932)	1:324:A:TYR:HA	1:325:A:GLY:H	20	0.26
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB2	5	0.26
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB3	5	0.26
(1,847)	1:313:A:CYS:HB2	1:314:A:ILE:HD11	19	0.26
(1,847)	1:313:A:CYS:HB2	1:314:A:ILE:HD12	19	0.26
(1,847)	1:313:A:CYS:HB2	1:314:A:ILE:HD13	19	0.26
(1,847)	1:313:A:CYS:HB3	1:314:A:ILE:HD11	19	0.26
(1,847)	1:313:A:CYS:HB3	1:314:A:ILE:HD12	19	0.26
(1,847)	1:313:A:CYS:HB3	1:314:A:ILE:HD13	19	0.26
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	20	0.26
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	20	0.26
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	19	0.26
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	17	0.26
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	11	0.26
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	11	0.26
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	11	0.26
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	20	0.26
(1,524)	1:241:A:ASN:HA	1:287:A:CYS:H	6	0.26
(1,484)	1:281:A:ILE:HA	1:282:A:LYS:H	3	0.26
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	5	0.26
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	15	0.26
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	10	0.26
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	2	0.26
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	2	0.26
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	2	0.26
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	1	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	9	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	9	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	14	0.26
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	14	0.26
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE2	8	0.26
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE3	8	0.26
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	18	0.26
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	18	0.26
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	14	0.25
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	8	0.25
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG21	8	0.25
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG22	8	0.25
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG23	8	0.25
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	14	0.25
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	14	0.25
(1,1671)	1:435:A:ARG:HG2	1:436:A:GLY:H	11	0.25
(1,1671)	1:435:A:ARG:HG3	1:436:A:GLY:H	11	0.25
(1,1671)	1:435:A:ARG:HG2	1:436:A:GLY:H	13	0.25
(1,1671)	1:435:A:ARG:HG3	1:436:A:GLY:H	13	0.25
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	16	0.25
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	16	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	16	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	16	0.25
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	17	0.25
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	17	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	17	0.25
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	17	0.25
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	12	0.25
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	12	0.25
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	12	0.25
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD11	16	0.25
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD12	16	0.25
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD13	16	0.25
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	8	0.25
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	8	0.25
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	3	0.25
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB2	12	0.25
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB3	12	0.25
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB2	12	0.25
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB3	12	0.25
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	14	0.25
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	14	0.25
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	14	0.25
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	14	0.25
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	14	0.25
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	14	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG11	20	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG12	20	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG13	20	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG21	20	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG22	20	0.25
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG23	20	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG11	10	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG12	10	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG13	10	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG21	10	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG22	10	0.25
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG23	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG11	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG12	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG13	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG21	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG22	10	0.25
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG23	10	0.25
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	2	0.25
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	7	0.25
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	7	0.25
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	7	0.25
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	7	0.25
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	7	0.25
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	7	0.25
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	8	0.25
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	8	0.25
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	10	0.25
(1,987)	1:324:A:TYR:HA	1:330:A:GLU:HA	5	0.25
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	2	0.25
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	2	0.25
(1,912)	1:322:A:ILE:HB	1:323:A:ILE:H	5	0.25
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	12	0.25
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	12	0.25
(1,898)	1:320:A:LYS:HB2	1:322:A:ILE:H	6	0.25
(1,898)	1:320:A:LYS:HB3	1:322:A:ILE:H	6	0.25
(1,890)	1:319:A:ASP:H	1:322:A:ILE:HD11	5	0.25
(1,890)	1:319:A:ASP:H	1:322:A:ILE:HD12	5	0.25
(1,890)	1:319:A:ASP:H	1:322:A:ILE:HD13	5	0.25
(1,866)	1:314:A:ILE:HG21	1:316:A:SER:H	2	0.25
(1,866)	1:314:A:ILE:HG22	1:316:A:SER:H	2	0.25
(1,866)	1:314:A:ILE:HG23	1:316:A:SER:H	2	0.25
(1,865)	1:239:A:ILE:HG21	1:316:A:SER:H	8	0.25
(1,865)	1:239:A:ILE:HG22	1:316:A:SER:H	8	0.25
(1,865)	1:239:A:ILE:HG23	1:316:A:SER:H	8	0.25
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	18	0.25
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	18	0.25
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	18	0.25
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	19	0.25
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	5	0.25
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	5	0.25
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	19	0.25
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	19	0.25
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	12	0.25
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	20	0.25
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	10	0.25
(1,514)	1:241:A:ASN:HA	1:286:A:ASP:H	14	0.25
(1,423)	1:277:A:LEU:H	1:279:A:PHE:H	2	0.25
(1,423)	1:277:A:LEU:H	1:279:A:PHE:H	11	0.25
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	1	0.25
(1,291)	1:265:A:LEU:HB2	1:266:A:ASP:H	9	0.25
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	9	0.25
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	9	0.25
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	7	0.25
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	7	0.25
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	7	0.25
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	7	0.25
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	7	0.25
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	13	0.25
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	13	0.25
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	13	0.25
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	12	0.25
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	12	0.25
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	12	0.25
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	12	0.25
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	11	0.24
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	11	0.24
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	7	0.24
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	7	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	5	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	5	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	5	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	11	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	11	0.24
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	11	0.24
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	11	0.24
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	11	0.24
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	11	0.24
(1,1781)	1:443:A:LEU:H	1:445:A:GLU:H	7	0.24
(1,1770)	1:443:A:LEU:HG	1:444:A:THR:H	17	0.24
(1,1748)	1:356:A:PHE:HE1	1:443:A:LEU:H	5	0.24
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB2	1	0.24
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB3	1	0.24
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB2	1	0.24
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB3	1	0.24
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	14	0.24
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	14	0.24
(1,1583)	1:424:A:SER:HA	1:428:A:SER:H	9	0.24
(1,1564)	1:424:A:SER:HB2	1:426:A:CYS:H	20	0.24
(1,1564)	1:424:A:SER:HB3	1:426:A:CYS:H	20	0.24
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	10	0.24
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	10	0.24
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	7	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD11	5	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD12	5	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD13	5	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD21	5	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD22	5	0.24
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD23	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD11	5	0.24
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD12	5	0.24
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD13	5	0.24
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD21	5	0.24
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD22	5	0.24
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD23	5	0.24
(1,1356)	1:373:A:THR:HB	1:381:A:LEU:HG	1	0.24
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	18	0.24
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	18	0.24
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	7	0.24
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	7	0.24
(1,1312)	1:248:A:ARG:HG2	1:373:A:THR:HB	4	0.24
(1,1312)	1:248:A:ARG:HG3	1:373:A:THR:HB	4	0.24
(1,1298)	1:370:A:PRO:HB2	1:371:A:VAL:H	18	0.24
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	11	0.24
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	1	0.24
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE2	15	0.24
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE3	15	0.24
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	15	0.24
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	15	0.24
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	8	0.24
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	19	0.24
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	19	0.24
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	19	0.24
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	8	0.24
(1,927)	1:324:A:TYR:H	1:324:A:TYR:HD1	9	0.24
(1,903)	1:322:A:ILE:H	1:322:A:ILE:HG13	8	0.24
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	16	0.24
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	16	0.24
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	17	0.24
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	3	0.24
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	18	0.24
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	9	0.24
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	15	0.24
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	20	0.24
(1,651)	1:294:A:GLU:H	1:297:A:LYS:H	11	0.24
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	4	0.24
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD11	11	0.24
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD12	11	0.24
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD13	11	0.24
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD11	11	0.24
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD12	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD13	11	0.24
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD11	11	0.24
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD12	11	0.24
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD13	11	0.24
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	14	0.24
(1,514)	1:241:A:ASN:HA	1:286:A:ASP:H	6	0.24
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	5	0.24
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	5	0.24
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	5	0.24
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD11	10	0.24
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD12	10	0.24
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD13	10	0.24
(1,427)	1:277:A:LEU:HD11	1:279:A:PHE:HE1	2	0.24
(1,427)	1:277:A:LEU:HD12	1:279:A:PHE:HE1	2	0.24
(1,427)	1:277:A:LEU:HD13	1:279:A:PHE:HE1	2	0.24
(1,427)	1:277:A:LEU:HD21	1:279:A:PHE:HE1	2	0.24
(1,427)	1:277:A:LEU:HD22	1:279:A:PHE:HE1	2	0.24
(1,427)	1:277:A:LEU:HD23	1:279:A:PHE:HE1	2	0.24
(1,423)	1:277:A:LEU:H	1:279:A:PHE:H	17	0.24
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG2	8	0.24
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG2	8	0.24
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG2	8	0.24
(1,385)	1:272:A:THR:HG21	1:276:A:GLU:HG3	8	0.24
(1,385)	1:272:A:THR:HG22	1:276:A:GLU:HG3	8	0.24
(1,385)	1:272:A:THR:HG23	1:276:A:GLU:HG3	8	0.24
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	1	0.24
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	11	0.24
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	11	0.24
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	11	0.24
(1,314)	1:267:A:ALA:HA	1:270:A:LEU:HG	14	0.24
(1,308)	1:266:A:ASP:H	1:269:A:ALA:H	12	0.24
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	13	0.24
(1,154)	1:247:A:ALA:HB1	1:248:A:ARG:H	19	0.24
(1,154)	1:247:A:ALA:HB2	1:248:A:ARG:H	19	0.24
(1,154)	1:247:A:ALA:HB3	1:248:A:ARG:H	19	0.24
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	10	0.23
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	15	0.23
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	15	0.23
(1,1969)	1:438:A:ASP:HB2	1:475:A:VAL:HB	18	0.23
(1,1969)	1:438:A:ASP:HB3	1:475:A:VAL:HB	18	0.23
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	13	0.23
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD11	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD12	3	0.23
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD13	3	0.23
(1,1919)	1:352:A:PRO:HA	1:474:A:LEU:HD11	14	0.23
(1,1919)	1:352:A:PRO:HA	1:474:A:LEU:HD12	14	0.23
(1,1919)	1:352:A:PRO:HA	1:474:A:LEU:HD13	14	0.23
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG11	1:473:A:LYS:HE3	16	0.23
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG12	1:473:A:LYS:HE3	16	0.23
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG13	1:473:A:LYS:HE3	16	0.23
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG21	1:473:A:LYS:HE3	16	0.23
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG22	1:473:A:LYS:HE3	16	0.23
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE2	16	0.23
(1,1901)	1:225:A:VAL:HG23	1:473:A:LYS:HE3	16	0.23
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD11	1	0.23
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD12	1	0.23
(1,1848)	1:440:A:LEU:HG	1:470:A:LEU:HD13	1	0.23
(1,1845)	1:400:A:LEU:HA	1:470:A:LEU:HG	6	0.23
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	15	0.23
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	20	0.23
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	20	0.23
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	20	0.23
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	20	0.23
(1,1807)	1:443:A:LEU:HD11	1:467:A:THR:H	18	0.23
(1,1807)	1:443:A:LEU:HD12	1:467:A:THR:H	18	0.23
(1,1807)	1:443:A:LEU:HD13	1:467:A:THR:H	18	0.23
(1,1807)	1:443:A:LEU:HD21	1:467:A:THR:H	18	0.23
(1,1807)	1:443:A:LEU:HD22	1:467:A:THR:H	18	0.23
(1,1807)	1:443:A:LEU:HD23	1:467:A:THR:H	18	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG11	7	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG12	7	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG13	7	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG21	7	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG22	7	0.23
(1,1792)	1:428:A:SER:H	1:446:A:VAL:HG23	7	0.23
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	17	0.23
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	17	0.23
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	17	0.23
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	17	0.23
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	17	0.23
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD11	16	0.23
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD12	16	0.23
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD13	16	0.23
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD11	4	0.23
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD12	4	0.23
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD13	4	0.23
(1,1719)	1:439:A:ILE:HG21	1:441:A:THR:H	19	0.23
(1,1719)	1:439:A:ILE:HG22	1:441:A:THR:H	19	0.23
(1,1719)	1:439:A:ILE:HG23	1:441:A:THR:H	19	0.23
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	4	0.23
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	4	0.23
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	4	0.23
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	4	0.23
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	4	0.23
(1,1638)	1:431:A:GLU:H	1:432:A:ARG:H	4	0.23
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	17	0.23
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	17	0.23
(1,1565)	1:424:A:SER:HA	1:426:A:CYS:H	9	0.23
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	2	0.23
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	2	0.23
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	2	0.23
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	2	0.23
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	2	0.23
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	2	0.23
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	13	0.23
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	13	0.23
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	13	0.23
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	20	0.23
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	20	0.23
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	20	0.23
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	7	0.23
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	7	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	8	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	8	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	8	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	8	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	8	0.23
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	8	0.23
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	8	0.23
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	8	0.23
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	8	0.23
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	8	0.23
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	8	0.23
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	1	0.23
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	2	0.23
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	2	0.23
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	2	0.23
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	2	0.23
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	3	0.23
(1,1349)	1:380:A:TYR:HA	1:380:A:TYR:HD1	5	0.23
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB1	13	0.23
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB2	13	0.23
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB3	13	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB1	13	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB2	13	0.23
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB3	13	0.23
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	17	0.23
(1,1127)	1:341:A:THR:H	1:344:A:LYS:HB2	15	0.23
(1,1127)	1:341:A:THR:H	1:344:A:LYS:HB3	15	0.23
(1,1086)	1:337:A:THR:HA	1:339:A:GLN:H	17	0.23
(1,1072)	1:336:A:LEU:HG	1:337:A:THR:H	11	0.23
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	17	0.23
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	18	0.23
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA2	15	0.23
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA3	15	0.23
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	4	0.23
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	4	0.23
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA2	14	0.23
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA3	14	0.23
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA2	14	0.23
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA3	14	0.23
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG12	17	0.23
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG13	17	0.23
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	1	0.23
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	1	0.23
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	4	0.23
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	4	0.23
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	1	0.23
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	1	0.23
(1,803)	1:309:A:CYS:HB2	1:310:A:PHE:H	11	0.23
(1,803)	1:309:A:CYS:HB3	1:310:A:PHE:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	16	0.23
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	3	0.23
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	3	0.23
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	14	0.23
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	7	0.23
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	7	0.23
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	7	0.23
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	7	0.23
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	7	0.23
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	7	0.23
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	7	0.23
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	7	0.23
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	7	0.23
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	7	0.23
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	20	0.23
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	17	0.23
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	17	0.23
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	17	0.23
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	16	0.23
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	13	0.23
(1,319)	1:269:A:ALA:HB1	1:270:A:LEU:HG	3	0.23
(1,319)	1:269:A:ALA:HB2	1:270:A:LEU:HG	3	0.23
(1,319)	1:269:A:ALA:HB3	1:270:A:LEU:HG	3	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD11	19	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD12	19	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD13	19	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD21	19	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD22	19	0.23
(1,283)	1:264:A:HIS:HD2	1:265:A:LEU:HD23	19	0.23
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	20	0.23
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	20	0.23
(1,281)	1:264:A:HIS:HD2	1:265:A:LEU:HG	14	0.23
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	4	0.23
(1,217)	1:251:A:VAL:HG21	1:254:A:LEU:HG	6	0.23
(1,217)	1:251:A:VAL:HG22	1:254:A:LEU:HG	6	0.23
(1,217)	1:251:A:VAL:HG23	1:254:A:LEU:HG	6	0.23
(1,211)	1:247:A:ALA:HB1	1:254:A:LEU:HG	4	0.23
(1,211)	1:247:A:ALA:HB2	1:254:A:LEU:HG	4	0.23
(1,211)	1:247:A:ALA:HB3	1:254:A:LEU:HG	4	0.23
(1,187)	1:247:A:ALA:HB1	1:251:A:VAL:H	4	0.23
(1,187)	1:247:A:ALA:HB2	1:251:A:VAL:H	4	0.23
(1,187)	1:247:A:ALA:HB3	1:251:A:VAL:H	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:248:A:ARG:HG2	1:249:A:GLU:H	14	0.23
(1,163)	1:248:A:ARG:HG3	1:249:A:GLU:H	14	0.23
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	19	0.23
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	19	0.23
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	2	0.23
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	2	0.23
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	2	0.23
(1,146)	1:245:A:ALA:H	1:247:A:ALA:H	19	0.23
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD2	15	0.23
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD3	15	0.23
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE2	11	0.23
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE3	11	0.23
(1,71)	1:232:A:PRO:HA	1:234:A:GLY:H	10	0.23
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	5	0.23
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	5	0.23
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	8	0.23
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	8	0.23
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	8	0.23
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	8	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	4	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	4	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	4	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	4	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	4	0.23
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	4	0.23
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	4	0.23
(1,7)	1:224:A:LYS:HB3	1:225:A:VAL:HB	12	0.23
(1,1942)	1:473:A:LYS:HE2	1:474:A:LEU:H	3	0.22
(1,1942)	1:473:A:LYS:HE3	1:474:A:LEU:H	3	0.22
(1,1933)	1:470:A:LEU:HD11	1:474:A:LEU:H	2	0.22
(1,1933)	1:470:A:LEU:HD12	1:474:A:LEU:H	2	0.22
(1,1933)	1:470:A:LEU:HD13	1:474:A:LEU:H	2	0.22
(1,1892)	1:225:A:VAL:HB	1:473:A:LYS:HA	12	0.22
(1,1770)	1:443:A:LEU:HG	1:444:A:THR:H	19	0.22
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD13	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD23	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD13	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD23	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD13	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD23	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD13	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD23	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD13	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD23	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD11	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD12	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD13	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD21	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD22	19	0.22
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD23	19	0.22
(1,1749)	1:356:A:PHE:HE1	1:443:A:LEU:HG	6	0.22
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG21	19	0.22
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG22	19	0.22
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG23	19	0.22
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	19	0.22
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	19	0.22
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	19	0.22
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG2	18	0.22
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG3	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB2	19	0.22
(1,1617)	1:429:A:LEU:HD11	1:430:A:ARG:HB3	19	0.22
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB2	19	0.22
(1,1617)	1:429:A:LEU:HD12	1:430:A:ARG:HB3	19	0.22
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB2	19	0.22
(1,1617)	1:429:A:LEU:HD13	1:430:A:ARG:HB3	19	0.22
(1,1564)	1:424:A:SER:HB2	1:426:A:CYS:H	3	0.22
(1,1564)	1:424:A:SER:HB3	1:426:A:CYS:H	3	0.22
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB2	17	0.22
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB3	17	0.22
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD11	6	0.22
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD12	6	0.22
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD13	6	0.22
(1,1517)	1:403:A:MET:HA	1:404:A:ALA:H	3	0.22
(1,1516)	1:403:A:MET:HG2	1:404:A:ALA:H	4	0.22
(1,1516)	1:403:A:MET:HG3	1:404:A:ALA:H	4	0.22
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	19	0.22
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	19	0.22
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	19	0.22
(1,1456)	1:398:A:ASP:H	1:399:A:PHE:HA	16	0.22
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	5	0.22
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	5	0.22
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	5	0.22
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	15	0.22
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	15	0.22
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	15	0.22
(1,1416)	1:320:A:LYS:HG2	1:392:A:TYR:HD1	17	0.22
(1,1416)	1:320:A:LYS:HG3	1:392:A:TYR:HD1	17	0.22
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	14	0.22
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	14	0.22
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	17	0.22
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	17	0.22
(1,1302)	1:370:A:PRO:HB2	1:371:A:VAL:HA	18	0.22
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	12	0.22
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	12	0.22
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	12	0.22
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	12	0.22
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	12	0.22
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	12	0.22
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	12	0.22
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	12	0.22
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG21	19	0.22
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG22	19	0.22
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG23	19	0.22
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG21	19	0.22
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG22	19	0.22
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG23	19	0.22
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG21	19	0.22
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG22	19	0.22
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG23	19	0.22
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	6	0.22
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	6	0.22
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	6	0.22
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	12	0.22
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	12	0.22
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	7	0.22
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	18	0.22
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	18	0.22
(1,945)	1:247:A:ALA:H	1:327:A:ASP:HB2	14	0.22
(1,945)	1:247:A:ALA:H	1:327:A:ASP:HB3	14	0.22
(1,944)	1:247:A:ALA:H	1:327:A:ASP:H	9	0.22
(1,885)	1:319:A:ASP:H	1:322:A:ILE:H	2	0.22
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	12	0.22
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	8	0.22
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	8	0.22
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	13	0.22
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	9	0.22
(1,706)	1:298:A:ILE:HD11	1:299:A:TYR:HE1	17	0.22
(1,706)	1:298:A:ILE:HD12	1:299:A:TYR:HE1	17	0.22
(1,706)	1:298:A:ILE:HD13	1:299:A:TYR:HE1	17	0.22
(1,705)	1:298:A:ILE:HG21	1:299:A:TYR:HE1	20	0.22
(1,705)	1:298:A:ILE:HG22	1:299:A:TYR:HE1	20	0.22
(1,705)	1:298:A:ILE:HG23	1:299:A:TYR:HE1	20	0.22
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	9	0.22
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	20	0.22
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	20	0.22
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	20	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	20	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	20	0.22
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	20	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	20	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	20	0.22
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	19	0.22
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	3	0.22
(1,500)	1:239:A:ILE:HG21	1:284:A:HIS:HB2	6	0.22
(1,500)	1:239:A:ILE:HG21	1:284:A:HIS:HB3	6	0.22
(1,500)	1:239:A:ILE:HG22	1:284:A:HIS:HB2	6	0.22
(1,500)	1:239:A:ILE:HG22	1:284:A:HIS:HB3	6	0.22
(1,500)	1:239:A:ILE:HG23	1:284:A:HIS:HB2	6	0.22
(1,500)	1:239:A:ILE:HG23	1:284:A:HIS:HB3	6	0.22
(1,465)	1:280:A:GLU:HB3	1:281:A:ILE:H	16	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD11	9	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD12	9	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD13	9	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD21	9	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD22	9	0.22
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD23	9	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG21	6	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG22	6	0.22
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG23	6	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG21	6	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG22	6	0.22
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG23	6	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG21	6	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG22	6	0.22
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG23	6	0.22
(1,310)	1:267:A:ALA:HA	1:269:A:ALA:H	3	0.22
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	12	0.22
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	12	0.22
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	12	0.22
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	3	0.22
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	3	0.22
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	3	0.22
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	16	0.22
(1,193)	1:250:A:LYS:HB2	1:251:A:VAL:H	11	0.22
(1,193)	1:250:A:LYS:HB3	1:251:A:VAL:H	11	0.22
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	1	0.22
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	1	0.22
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	11	0.22
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	11	0.22
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	11	0.22
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	20	0.22
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	20	0.22
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	15	0.22
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	15	0.22
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	12	0.21
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	15	0.21
(1,1983)	1:228:A:MET:HE1	1:476:A:PHE:HE1	15	0.21
(1,1983)	1:228:A:MET:HE2	1:476:A:PHE:HE1	15	0.21
(1,1983)	1:228:A:MET:HE3	1:476:A:PHE:HE1	15	0.21
(1,1980)	1:474:A:LEU:HD11	1:475:A:VAL:H	15	0.21
(1,1980)	1:474:A:LEU:HD12	1:475:A:VAL:H	15	0.21
(1,1980)	1:474:A:LEU:HD13	1:475:A:VAL:H	15	0.21
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	7	0.21
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG2	16	0.21
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG3	16	0.21
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG3	16	0.21
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG3	16	0.21
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG3	16	0.21
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG3	16	0.21
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG3	16	0.21
(1,1858)	1:469:A:THR:HA	1:470:A:LEU:HA	12	0.21
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	8	0.21
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG21	13	0.21
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG22	13	0.21
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG23	13	0.21
(1,1759)	1:439:A:ILE:HA	1:443:A:LEU:H	5	0.21
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD11	20	0.21
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD12	20	0.21
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD13	20	0.21
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB2	7	0.21
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB3	7	0.21
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	3	0.21
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	3	0.21
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	8	0.21
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	8	0.21
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	11	0.21
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	11	0.21
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	2	0.21
(1,1613)	1:427:A:GLN:HA	1:430:A:ARG:HD2	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1613)	1:427:A:GLN:HA	1:430:A:ARG:HD3	10	0.21
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	13	0.21
(1,1540)	1:423:A:GLN:H	1:424:A:SER:H	1	0.21
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	8	0.21
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	8	0.21
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	8	0.21
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	8	0.21
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	8	0.21
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	8	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD11	15	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD12	15	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD13	15	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD21	15	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD22	15	0.21
(1,1458)	1:311:A:ILE:HG21	1:400:A:LEU:HD23	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD11	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD12	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD13	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD21	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD22	15	0.21
(1,1458)	1:311:A:ILE:HG22	1:400:A:LEU:HD23	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD11	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD12	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD13	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD21	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD22	15	0.21
(1,1458)	1:311:A:ILE:HG23	1:400:A:LEU:HD23	15	0.21
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG21	10	0.21
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG22	10	0.21
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG23	10	0.21
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG21	10	0.21
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG22	10	0.21
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG23	10	0.21
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	18	0.21
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	18	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	19	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	19	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	19	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	19	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	19	0.21
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	19	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	19	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	19	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	19	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	19	0.21
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	19	0.21
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	1	0.21
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	1	0.21
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	1	0.21
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	1	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	1	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	1	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	1	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	1	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	11	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	11	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	11	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	11	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	16	0.21
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	16	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	16	0.21
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	16	0.21
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	9	0.21
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	9	0.21
(1,1315)	1:373:A:THR:HB	1:374:A:ASP:HA	12	0.21
(1,1289)	1:369:A:ILE:HD11	1:370:A:PRO:HG2	20	0.21
(1,1289)	1:369:A:ILE:HD11	1:370:A:PRO:HG3	20	0.21
(1,1289)	1:369:A:ILE:HD12	1:370:A:PRO:HG2	20	0.21
(1,1289)	1:369:A:ILE:HD12	1:370:A:PRO:HG3	20	0.21
(1,1289)	1:369:A:ILE:HD13	1:370:A:PRO:HG2	20	0.21
(1,1289)	1:369:A:ILE:HD13	1:370:A:PRO:HG3	20	0.21
(1,1274)	1:368:A:GLY:HA2	1:369:A:ILE:HG12	1	0.21
(1,1274)	1:368:A:GLY:HA3	1:369:A:ILE:HG12	1	0.21
(1,1233)	1:312:A:CYS:H	1:356:A:PHE:H	16	0.21
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	17	0.21
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	15	0.21
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	20	0.21
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	20	0.21
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	17	0.21
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	11	0.21
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	11	0.21
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	11	0.21
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	11	0.21
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	11	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	8	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	8	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	8	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	15	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	15	0.21
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	15	0.21
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG23	11	0.21
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG23	11	0.21
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG23	11	0.21
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG23	11	0.21
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG23	11	0.21
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG21	11	0.21
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG22	11	0.21
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG23	11	0.21
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	3	0.21
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	3	0.21
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	8	0.21
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	8	0.21
(1,925)	1:323:A:ILE:HB	1:324:A:TYR:H	13	0.21
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG12	1	0.21
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG13	1	0.21
(1,885)	1:319:A:ASP:H	1:322:A:ILE:H	10	0.21
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	5	0.21
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	5	0.21
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	1	0.21
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	1	0.21
(1,812)	1:310:A:PHE:HD1	1:311:A:ILE:H	10	0.21
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	17	0.21
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	18	0.21
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	3	0.21
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	3	0.21
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	1	0.21
(1,651)	1:294:A:GLU:H	1:297:A:LYS:H	12	0.21
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	14	0.21
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	14	0.21
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	14	0.21
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	14	0.21
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	14	0.21
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	14	0.21
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	14	0.21
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	14	0.21
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	14	0.21
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	7	0.21
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	10	0.21
(1,550)	1:287:A:CYS:HB2	1:291:A:GLN:H	2	0.21
(1,550)	1:287:A:CYS:HB3	1:291:A:GLN:H	2	0.21
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	3	0.21
(1,469)	1:280:A:GLU:HB3	1:281:A:ILE:HA	7	0.21
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	12	0.21
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	12	0.21
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	12	0.21
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	10	0.21
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	10	0.21
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	10	0.21
(1,448)	1:238:A:ILE:HD11	1:281:A:ILE:HA	18	0.21
(1,448)	1:238:A:ILE:HD12	1:281:A:ILE:HA	18	0.21
(1,448)	1:238:A:ILE:HD13	1:281:A:ILE:HA	18	0.21
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	9	0.21
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	9	0.21
(1,425)	1:277:A:LEU:HG	1:279:A:PHE:HE1	11	0.21
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG21	3	0.21
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG22	3	0.21
(1,326)	1:238:A:ILE:HD11	1:271:A:THR:HG23	3	0.21
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG21	3	0.21
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG22	3	0.21
(1,326)	1:238:A:ILE:HD12	1:271:A:THR:HG23	3	0.21
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG21	3	0.21
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG22	3	0.21
(1,326)	1:238:A:ILE:HD13	1:271:A:THR:HG23	3	0.21
(1,325)	1:238:A:ILE:HD11	1:271:A:THR:HB	2	0.21
(1,325)	1:238:A:ILE:HD12	1:271:A:THR:HB	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:238:A:ILE:HD13	1:271:A:THR:HB	2	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD11	9	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD12	9	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD13	9	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD21	9	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD22	9	0.21
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD23	9	0.21
(1,276)	1:258:A:ARG:H	1:259:A:ASP:HA	17	0.21
(1,240)	1:255:A:HIS:H	1:255:A:HIS:HD2	17	0.21
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	5	0.21
(1,228)	1:253:A:LYS:HD2	1:254:A:LEU:HD21	18	0.21
(1,228)	1:253:A:LYS:HD2	1:254:A:LEU:HD22	18	0.21
(1,228)	1:253:A:LYS:HD2	1:254:A:LEU:HD23	18	0.21
(1,228)	1:253:A:LYS:HD3	1:254:A:LEU:HD21	18	0.21
(1,228)	1:253:A:LYS:HD3	1:254:A:LEU:HD22	18	0.21
(1,228)	1:253:A:LYS:HD3	1:254:A:LEU:HD23	18	0.21
(1,212)	1:247:A:ALA:HB1	1:254:A:LEU:HD11	6	0.21
(1,212)	1:247:A:ALA:HB1	1:254:A:LEU:HD12	6	0.21
(1,212)	1:247:A:ALA:HB1	1:254:A:LEU:HD13	6	0.21
(1,212)	1:247:A:ALA:HB2	1:254:A:LEU:HD11	6	0.21
(1,212)	1:247:A:ALA:HB2	1:254:A:LEU:HD12	6	0.21
(1,212)	1:247:A:ALA:HB2	1:254:A:LEU:HD13	6	0.21
(1,212)	1:247:A:ALA:HB3	1:254:A:LEU:HD11	6	0.21
(1,212)	1:247:A:ALA:HB3	1:254:A:LEU:HD12	6	0.21
(1,212)	1:247:A:ALA:HB3	1:254:A:LEU:HD13	6	0.21
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	10	0.21
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	10	0.21
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	10	0.21
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	10	0.21
(1,100)	1:239:A:ILE:H	1:239:A:ILE:HD11	2	0.21
(1,100)	1:239:A:ILE:H	1:239:A:ILE:HD12	2	0.21
(1,100)	1:239:A:ILE:H	1:239:A:ILE:HD13	2	0.21
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	12	0.21
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	4	0.21
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	20	0.21
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	20	0.21
(1,38)	1:228:A:MET:HA	1:229:A:LYS:H	8	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	9	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	9	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	9	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	9	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	9	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	9	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	17	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	17	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	17	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	17	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	17	0.21
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	17	0.21
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	17	0.21
(1,7)	1:224:A:LYS:HB3	1:225:A:VAL:HB	8	0.21
(1,2019)	1:477:A:PRO:HB2	1:479:A:ASP:H	12	0.2
(1,1989)	1:354:A:VAL:HG11	1:476:A:PHE:HZ	12	0.2
(1,1989)	1:354:A:VAL:HG12	1:476:A:PHE:HZ	12	0.2
(1,1989)	1:354:A:VAL:HG13	1:476:A:PHE:HZ	12	0.2
(1,1989)	1:354:A:VAL:HG21	1:476:A:PHE:HZ	12	0.2
(1,1989)	1:354:A:VAL:HG22	1:476:A:PHE:HZ	12	0.2
(1,1989)	1:354:A:VAL:HG23	1:476:A:PHE:HZ	12	0.2
(1,1988)	1:311:A:ILE:HG21	1:476:A:PHE:HZ	11	0.2
(1,1988)	1:311:A:ILE:HG22	1:476:A:PHE:HZ	11	0.2
(1,1988)	1:311:A:ILE:HG23	1:476:A:PHE:HZ	11	0.2
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	3	0.2
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	3	0.2
(1,1974)	1:473:A:LYS:HG3	1:475:A:VAL:HB	19	0.2
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG11	2	0.2
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG12	2	0.2
(1,1962)	1:438:A:ASP:HA	1:475:A:VAL:HG13	2	0.2
(1,1858)	1:469:A:THR:HA	1:470:A:LEU:HA	14	0.2
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	8	0.2
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	8	0.2
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	8	0.2
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG21	11	0.2
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG22	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG23	11	0.2
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG21	20	0.2
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG22	20	0.2
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG23	20	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	1	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	1	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	1	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	8	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	8	0.2
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	8	0.2
(1,1822)	1:399:A:PHE:H	1:469:A:THR:H	16	0.2
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	14	0.2
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD11	11	0.2
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD12	11	0.2
(1,1740)	1:441:A:THR:H	1:442:A:ILE:HD13	11	0.2
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD11	16	0.2
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD12	16	0.2
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD13	16	0.2
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	17	0.2
(1,1686)	1:311:A:ILE:HD11	1:439:A:ILE:HG21	5	0.2
(1,1686)	1:311:A:ILE:HD11	1:439:A:ILE:HG22	5	0.2
(1,1686)	1:311:A:ILE:HD11	1:439:A:ILE:HG23	5	0.2
(1,1686)	1:311:A:ILE:HD12	1:439:A:ILE:HG21	5	0.2
(1,1686)	1:311:A:ILE:HD12	1:439:A:ILE:HG22	5	0.2
(1,1686)	1:311:A:ILE:HD12	1:439:A:ILE:HG23	5	0.2
(1,1686)	1:311:A:ILE:HD13	1:439:A:ILE:HG21	5	0.2
(1,1686)	1:311:A:ILE:HD13	1:439:A:ILE:HG22	5	0.2
(1,1686)	1:311:A:ILE:HD13	1:439:A:ILE:HG23	5	0.2
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA2	13	0.2
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA3	13	0.2
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG2	19	0.2
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG3	19	0.2
(1,1548)	1:422:A:ILE:H	1:425:A:LEU:H	7	0.2
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD11	11	0.2
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD12	11	0.2
(1,1530)	1:422:A:ILE:HA	1:422:A:ILE:HD13	11	0.2
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	5	0.2
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	5	0.2
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	5	0.2
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	5	0.2
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	5	0.2
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:403:A:MET:HG2	1:404:A:ALA:H	7	0.2
(1,1516)	1:403:A:MET:HG3	1:404:A:ALA:H	7	0.2
(1,1482)	1:400:A:LEU:HG	1:401:A:LEU:H	11	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	20	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	20	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	20	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	20	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	20	0.2
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	20	0.2
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	20	0.2
(1,1397)	1:384:A:ASP:HA	1:385:A:LEU:HA	16	0.2
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	7	0.2
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	7	0.2
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	7	0.2
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	7	0.2
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	18	0.2
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	18	0.2
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	18	0.2
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	18	0.2
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	4	0.2
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	19	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD11	9	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD12	9	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD13	9	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD21	9	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD22	9	0.2
(1,1362)	1:376:A:GLU:HB2	1:381:A:LEU:HD23	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD11	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD12	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD13	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD21	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD22	9	0.2
(1,1362)	1:376:A:GLU:HB3	1:381:A:LEU:HD23	9	0.2
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB2	9	0.2
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB3	9	0.2
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	3	0.2
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	3	0.2
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	3	0.2
(1,1320)	1:248:A:ARG:HD2	1:376:A:GLU:HA	16	0.2
(1,1320)	1:248:A:ARG:HD3	1:376:A:GLU:HA	16	0.2
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	5	0.2
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	5	0.2
(1,1297)	1:369:A:ILE:HD11	1:371:A:VAL:HA	20	0.2
(1,1297)	1:369:A:ILE:HD12	1:371:A:VAL:HA	20	0.2
(1,1297)	1:369:A:ILE:HD13	1:371:A:VAL:HA	20	0.2
(1,1267)	1:360:A:ALA:HB1	1:361:A:GLN:HA	6	0.2
(1,1267)	1:360:A:ALA:HB2	1:361:A:GLN:HA	6	0.2
(1,1267)	1:360:A:ALA:HB3	1:361:A:GLN:HA	6	0.2
(1,1255)	1:357:A:ILE:HG21	1:359:A:ALA:HA	5	0.2
(1,1255)	1:357:A:ILE:HG22	1:359:A:ALA:HA	5	0.2
(1,1255)	1:357:A:ILE:HG23	1:359:A:ALA:HA	5	0.2
(1,1236)	1:314:A:ILE:H	1:356:A:PHE:H	15	0.2
(1,1232)	1:311:A:ILE:HG21	1:356:A:PHE:HE1	7	0.2
(1,1232)	1:311:A:ILE:HG22	1:356:A:PHE:HE1	7	0.2
(1,1232)	1:311:A:ILE:HG23	1:356:A:PHE:HE1	7	0.2
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	20	0.2
(1,1172)	1:348:A:LEU:H	1:348:A:LEU:HG	19	0.2
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	19	0.2
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	19	0.2
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	4	0.2
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	19	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	13	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	13	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	13	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	13	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	13	0.2
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	13	0.2
(1,1110)	1:341:A:THR:HB	1:343:A:LEU:HG	8	0.2
(1,1075)	1:296:A:LEU:HD11	1:338:A:SER:H	13	0.2
(1,1075)	1:296:A:LEU:HD12	1:338:A:SER:H	13	0.2
(1,1075)	1:296:A:LEU:HD13	1:338:A:SER:H	13	0.2
(1,1075)	1:296:A:LEU:HD21	1:338:A:SER:H	13	0.2
(1,1075)	1:296:A:LEU:HD22	1:338:A:SER:H	13	0.2
(1,1075)	1:296:A:LEU:HD23	1:338:A:SER:H	13	0.2
(1,1068)	1:336:A:LEU:HD11	1:337:A:THR:H	11	0.2
(1,1068)	1:336:A:LEU:HD12	1:337:A:THR:H	11	0.2
(1,1068)	1:336:A:LEU:HD13	1:337:A:THR:H	11	0.2
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	20	0.2
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	20	0.2
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	20	0.2
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	4	0.2
(1,931)	1:324:A:TYR:HB2	1:325:A:GLY:H	3	0.2
(1,889)	1:319:A:ASP:H	1:322:A:ILE:HG12	12	0.2
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	1	0.2
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	1	0.2
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	14	0.2
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	14	0.2
(1,828)	1:311:A:ILE:HD11	1:312:A:CYS:H	6	0.2
(1,828)	1:311:A:ILE:HD12	1:312:A:CYS:H	6	0.2
(1,828)	1:311:A:ILE:HD13	1:312:A:CYS:H	6	0.2
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	11	0.2
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	11	0.2
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	7	0.2
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	7	0.2
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	7	0.2
(1,747)	1:300:A:GLN:H	1:302:A:MET:H	2	0.2
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	4	0.2
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	4	0.2
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	4	0.2
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	5	0.2
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	5	0.2
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	5	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD11	6	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD12	6	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD13	6	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD21	6	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD22	6	0.2
(1,721)	1:297:A:LYS:HG2	1:301:A:LEU:HD23	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD11	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD12	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD13	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD21	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD22	6	0.2
(1,721)	1:297:A:LYS:HG3	1:301:A:LEU:HD23	6	0.2
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	4	0.2
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	6	0.2
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	4	0.2
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	4	0.2
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:297:A:LYS:HA	1:299:A:TYR:H	13	0.2
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	10	0.2
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	13	0.2
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	19	0.2
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB2	18	0.2
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB3	18	0.2
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	14	0.2
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD11	13	0.2
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD12	13	0.2
(1,464)	1:279:A:PHE:HD1	1:281:A:ILE:HD13	13	0.2
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG12	17	0.2
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG13	17	0.2
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	7	0.2
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	7	0.2
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB2	17	0.2
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB3	17	0.2
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	8	0.2
(1,413)	1:276:A:GLU:H	1:278:A:HIS:H	3	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD11	15	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD12	15	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD13	15	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD21	15	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD22	15	0.2
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD23	15	0.2
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	15	0.2
(1,345)	1:270:A:LEU:HA	1:273:A:THR:H	12	0.2
(1,333)	1:269:A:ALA:HA	1:272:A:THR:H	11	0.2
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	5	0.2
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	16	0.2
(1,281)	1:264:A:HIS:HD2	1:265:A:LEU:HG	5	0.2
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD3	5	0.2
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD3	5	0.2
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD3	5	0.2
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD3	5	0.2
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD3	5	0.2
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD2	5	0.2
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	2	0.2
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	9	0.2
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD2	5	0.2
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD3	5	0.2
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	11	0.2
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	11	0.2
(1,48)	1:229:A:LYS:HG2	1:230:A:SER:H	3	0.2
(1,48)	1:229:A:LYS:HG3	1:230:A:SER:H	3	0.2
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	15	0.2
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	15	0.2
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	4	0.19
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	4	0.19
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	4	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD11	19	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD12	19	0.19
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD13	19	0.19
(1,1865)	1:398:A:ASP:H	1:471:A:ARG:HD2	5	0.19
(1,1865)	1:398:A:ASP:H	1:471:A:ARG:HD3	5	0.19
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD11	7	0.19
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD12	7	0.19
(1,1846)	1:400:A:LEU:HA	1:470:A:LEU:HD13	7	0.19
(1,1845)	1:400:A:LEU:HA	1:470:A:LEU:HG	2	0.19
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	3	0.19
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	3	0.19
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	3	0.19
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	13	0.19
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	13	0.19
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	13	0.19
(1,1816)	1:467:A:THR:HA	1:468:A:PHE:H	4	0.19
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	11	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD23	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD23	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD23	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD23	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD23	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD11	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD12	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD13	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD21	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD22	6	0.19
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD23	6	0.19
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	8	0.19
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	8	0.19
(1,1633)	1:430:A:ARG:HG2	1:431:A:GLU:H	7	0.19
(1,1633)	1:430:A:ARG:HG3	1:431:A:GLU:H	7	0.19
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	16	0.19
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	16	0.19
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	16	0.19
(1,1588)	1:427:A:GLN:HG2	1:428:A:SER:HA	10	0.19
(1,1588)	1:427:A:GLN:HG3	1:428:A:SER:HA	10	0.19
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE1	18	0.19
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE2	18	0.19
(1,1506)	1:392:A:TYR:HD1	1:403:A:MET:HE3	18	0.19
(1,1482)	1:400:A:LEU:HG	1:401:A:LEU:H	16	0.19
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	6	0.19
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	6	0.19
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	18	0.19
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD11	4	0.19
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD12	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD13	4	0.19
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD21	4	0.19
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD22	4	0.19
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD23	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD11	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD12	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD13	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD21	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD22	4	0.19
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD23	4	0.19
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB2	13	0.19
(1,1348)	1:380:A:TYR:H	1:380:A:TYR:HB3	13	0.19
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	8	0.19
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	8	0.19
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	8	0.19
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	8	0.19
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	18	0.19
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	18	0.19
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	18	0.19
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	18	0.19
(1,1302)	1:370:A:PRO:HB2	1:371:A:VAL:HA	5	0.19
(1,1226)	1:354:A:VAL:HG11	1:355:A:PHE:H	11	0.19
(1,1226)	1:354:A:VAL:HG12	1:355:A:PHE:H	11	0.19
(1,1226)	1:354:A:VAL:HG13	1:355:A:PHE:H	11	0.19
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	18	0.19
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	18	0.19
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	18	0.19
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	18	0.19
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	18	0.19
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	18	0.19
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	1	0.19
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	1	0.19
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	9	0.19
(1,1085)	1:337:A:THR:H	1:339:A:GLN:H	10	0.19
(1,1066)	1:335:A:GLU:H	1:337:A:THR:H	6	0.19
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	4	0.19
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	4	0.19
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	4	0.19
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	11	0.19
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	11	0.19
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	11	0.19
(1,1009)	1:333:A:ILE:HG21	1:334:A:TYR:HB2	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:333:A:ILE:HG22	1:334:A:TYR:HB2	3	0.19
(1,1009)	1:333:A:ILE:HG23	1:334:A:TYR:HB2	3	0.19
(1,983)	1:289:A:VAL:HB	1:330:A:GLU:H	15	0.19
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	5	0.19
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	5	0.19
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	18	0.19
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	18	0.19
(1,910)	1:322:A:ILE:HA	1:323:A:ILE:H	13	0.19
(1,910)	1:322:A:ILE:HA	1:323:A:ILE:H	15	0.19
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	19	0.19
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	19	0.19
(1,888)	1:319:A:ASP:H	1:322:A:ILE:HG21	5	0.19
(1,888)	1:319:A:ASP:H	1:322:A:ILE:HG22	5	0.19
(1,888)	1:319:A:ASP:H	1:322:A:ILE:HG23	5	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	19	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	19	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	19	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	20	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	20	0.19
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	20	0.19
(1,795)	1:307:A:MET:HE1	1:309:A:CYS:H	12	0.19
(1,795)	1:307:A:MET:HE2	1:309:A:CYS:H	12	0.19
(1,795)	1:307:A:MET:HE3	1:309:A:CYS:H	12	0.19
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	1	0.19
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	15	0.19
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	5	0.19
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	5	0.19
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	5	0.19
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	5	0.19
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	16	0.19
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	13	0.19
(1,550)	1:287:A:CYS:HB2	1:291:A:GLN:H	7	0.19
(1,550)	1:287:A:CYS:HB3	1:291:A:GLN:H	7	0.19
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	15	0.19
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	15	0.19
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	15	0.19
(1,538)	1:288:A:THR:HA	1:290:A:GLU:H	12	0.19
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	6	0.19
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	14	0.19
(1,501)	1:240:A:ASN:HB2	1:284:A:HIS:H	12	0.19
(1,501)	1:240:A:ASN:HB3	1:284:A:HIS:H	12	0.19
(1,445)	1:236:A:CYS:H	1:281:A:ILE:HA	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	14	0.19
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	14	0.19
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	10	0.19
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	11	0.19
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	6	0.19
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	9	0.19
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG2	2	0.19
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG3	2	0.19
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG2	3	0.19
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG3	3	0.19
(1,281)	1:264:A:HIS:HD2	1:265:A:LEU:HG	9	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	3	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	3	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	3	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	5	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	5	0.19
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	5	0.19
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	15	0.19
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	15	0.19
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	15	0.19
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	8	0.19
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD21	7	0.19
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD22	7	0.19
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD23	7	0.19
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD21	7	0.19
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD22	7	0.19
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD23	7	0.19
(1,224)	1:251:A:VAL:HG11	1:254:A:LEU:HG	6	0.19
(1,224)	1:251:A:VAL:HG12	1:254:A:LEU:HG	6	0.19
(1,224)	1:251:A:VAL:HG13	1:254:A:LEU:HG	6	0.19
(1,224)	1:251:A:VAL:HG21	1:254:A:LEU:HG	6	0.19
(1,224)	1:251:A:VAL:HG22	1:254:A:LEU:HG	6	0.19
(1,224)	1:251:A:VAL:HG23	1:254:A:LEU:HG	6	0.19
(1,217)	1:251:A:VAL:HG21	1:254:A:LEU:HG	18	0.19
(1,217)	1:251:A:VAL:HG22	1:254:A:LEU:HG	18	0.19
(1,217)	1:251:A:VAL:HG23	1:254:A:LEU:HG	18	0.19
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD2	18	0.19
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD3	18	0.19
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD3	11	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD3	11	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD3	11	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD3	11	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD2	11	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD3	11	0.19
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD3	19	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD3	19	0.19
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD3	19	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD3	19	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD3	19	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD2	19	0.19
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD3	19	0.19
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG2	18	0.19
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG3	18	0.19
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG2	18	0.19
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG3	18	0.19
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	8	0.19
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	12	0.19
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	12	0.19
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	12	0.19
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD2	4	0.19
(1,138)	1:246:A:LYS:HA	1:246:A:LYS:HD3	4	0.19
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	17	0.19
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	9	0.19
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	9	0.19
(1,2017)	1:277:A:LEU:HD11	1:479:A:ASP:H	7	0.18
(1,2017)	1:277:A:LEU:HD12	1:479:A:ASP:H	7	0.18
(1,2017)	1:277:A:LEU:HD13	1:479:A:ASP:H	7	0.18
(1,2017)	1:277:A:LEU:HD21	1:479:A:ASP:H	7	0.18
(1,2017)	1:277:A:LEU:HD22	1:479:A:ASP:H	7	0.18
(1,2017)	1:277:A:LEU:HD23	1:479:A:ASP:H	7	0.18
(1,2000)	1:475:A:VAL:HB	1:476:A:PHE:HA	3	0.18
(1,1992)	1:439:A:ILE:HG21	1:476:A:PHE:HE1	8	0.18
(1,1992)	1:439:A:ILE:HG22	1:476:A:PHE:HE1	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1992)	1:439:A:ILE:HG23	1:476:A:PHE:HE1	8	0.18
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	8	0.18
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	8	0.18
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	8	0.18
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG11	1:473:A:LYS:HD3	17	0.18
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG12	1:473:A:LYS:HD3	17	0.18
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG13	1:473:A:LYS:HD3	17	0.18
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG21	1:473:A:LYS:HD3	17	0.18
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG22	1:473:A:LYS:HD3	17	0.18
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD2	17	0.18
(1,1900)	1:225:A:VAL:HG23	1:473:A:LYS:HD3	17	0.18
(1,1858)	1:469:A:THR:HA	1:470:A:LEU:HA	7	0.18
(1,1845)	1:400:A:LEU:HA	1:470:A:LEU:HG	8	0.18
(1,1822)	1:399:A:PHE:H	1:469:A:THR:H	11	0.18
(1,1820)	1:397:A:ALA:HB1	1:469:A:THR:HB	15	0.18
(1,1820)	1:397:A:ALA:HB2	1:469:A:THR:HB	15	0.18
(1,1820)	1:397:A:ALA:HB3	1:469:A:THR:HB	15	0.18
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	6	0.18
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	6	0.18
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	6	0.18
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	10	0.18
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	10	0.18
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	10	0.18
(1,1816)	1:467:A:THR:HA	1:468:A:PHE:H	11	0.18
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	7	0.18
(1,1795)	1:444:A:THR:HG21	1:446:A:VAL:H	15	0.18
(1,1795)	1:444:A:THR:HG22	1:446:A:VAL:H	15	0.18
(1,1795)	1:444:A:THR:HG23	1:446:A:VAL:H	15	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	10	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	16	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	16	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	16	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	16	0.18
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	16	0.18
(1,1748)	1:356:A:PHE:HE1	1:443:A:LEU:H	20	0.18
(1,1640)	1:273:A:THR:HG21	1:433:A:CYS:H	2	0.18
(1,1640)	1:273:A:THR:HG22	1:433:A:CYS:H	2	0.18
(1,1640)	1:273:A:THR:HG23	1:433:A:CYS:H	2	0.18
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	6	0.18
(1,1564)	1:424:A:SER:HB2	1:426:A:CYS:H	14	0.18
(1,1564)	1:424:A:SER:HB3	1:426:A:CYS:H	14	0.18
(1,1516)	1:403:A:MET:HG2	1:404:A:ALA:H	10	0.18
(1,1516)	1:403:A:MET:HG3	1:404:A:ALA:H	10	0.18
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	12	0.18
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	12	0.18
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	15	0.18
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	15	0.18
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	3	0.18
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	3	0.18
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	13	0.18
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	13	0.18
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	2	0.18
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	12	0.18
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	12	0.18
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	12	0.18
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	12	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	13	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	13	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	13	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	13	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	13	0.18
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	13	0.18
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	4	0.18
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	4	0.18
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	4	0.18
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	4	0.18
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	4	0.18
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	4	0.18
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	14	0.18
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	14	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	14	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	14	0.18
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	19	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	19	0.18
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	19	0.18
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB2	19	0.18
(1,1341)	1:376:A:GLU:HA	1:380:A:TYR:HB3	19	0.18
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	7	0.18
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	7	0.18
(1,1315)	1:373:A:THR:HB	1:374:A:ASP:HA	13	0.18
(1,1252)	1:357:A:ILE:HG21	1:358:A:GLN:HA	17	0.18
(1,1252)	1:357:A:ILE:HG22	1:358:A:GLN:HA	17	0.18
(1,1252)	1:357:A:ILE:HG23	1:358:A:GLN:HA	17	0.18
(1,1233)	1:312:A:CYS:H	1:356:A:PHE:H	20	0.18
(1,1206)	1:311:A:ILE:HG21	1:354:A:VAL:HG21	15	0.18
(1,1206)	1:311:A:ILE:HG21	1:354:A:VAL:HG22	15	0.18
(1,1206)	1:311:A:ILE:HG21	1:354:A:VAL:HG23	15	0.18
(1,1206)	1:311:A:ILE:HG22	1:354:A:VAL:HG21	15	0.18
(1,1206)	1:311:A:ILE:HG22	1:354:A:VAL:HG22	15	0.18
(1,1206)	1:311:A:ILE:HG22	1:354:A:VAL:HG23	15	0.18
(1,1206)	1:311:A:ILE:HG23	1:354:A:VAL:HG21	15	0.18
(1,1206)	1:311:A:ILE:HG23	1:354:A:VAL:HG22	15	0.18
(1,1206)	1:311:A:ILE:HG23	1:354:A:VAL:HG23	15	0.18
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	9	0.18
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	13	0.18
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	13	0.18
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB2	17	0.18
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB3	17	0.18
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	7	0.18
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	7	0.18
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	7	0.18
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	5	0.18
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	5	0.18
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	5	0.18
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	1	0.18
(1,1015)	1:334:A:TYR:HA	1:334:A:TYR:HD1	19	0.18
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	3	0.18
(1,932)	1:324:A:TYR:HA	1:325:A:GLY:H	13	0.18
(1,865)	1:239:A:ILE:HG21	1:316:A:SER:H	16	0.18
(1,865)	1:239:A:ILE:HG22	1:316:A:SER:H	16	0.18
(1,865)	1:239:A:ILE:HG23	1:316:A:SER:H	16	0.18
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	4	0.18
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	4	0.18
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:302:A:MET:H	1:303:A:ASP:HA	20	0.18
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	12	0.18
(1,714)	1:298:A:ILE:H	1:300:A:GLN:H	14	0.18
(1,709)	1:299:A:TYR:H	1:299:A:TYR:HE1	9	0.18
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	12	0.18
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	12	0.18
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	12	0.18
(1,697)	1:297:A:LYS:HA	1:299:A:TYR:H	16	0.18
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	9	0.18
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	9	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	9	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	9	0.18
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	17	0.18
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	17	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	17	0.18
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	17	0.18
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	2	0.18
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	2	0.18
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	2	0.18
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	18	0.18
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	18	0.18
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	18	0.18
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	18	0.18
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	18	0.18
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	18	0.18
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	18	0.18
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	18	0.18
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	18	0.18
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD11	6	0.18
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD12	6	0.18
(1,623)	1:292:A:ILE:HG21	1:295:A:ILE:HD13	6	0.18
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD11	6	0.18
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD12	6	0.18
(1,623)	1:292:A:ILE:HG22	1:295:A:ILE:HD13	6	0.18
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD11	6	0.18
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD12	6	0.18
(1,623)	1:292:A:ILE:HG23	1:295:A:ILE:HD13	6	0.18
(1,534)	1:288:A:THR:HB	1:289:A:VAL:H	7	0.18
(1,518)	1:242:A:HIS:H	1:286:A:ASP:H	18	0.18
(1,517)	1:242:A:HIS:H	1:286:A:ASP:HA	6	0.18
(1,506)	1:240:A:ASN:H	1:285:A:ASP:HA	18	0.18
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	18	0.18
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD11	4	0.18
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD12	4	0.18
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD13	4	0.18
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	3	0.18
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	3	0.18
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	3	0.18
(1,437)	1:235:A:TYR:HB2	1:280:A:GLU:HB2	16	0.18
(1,437)	1:235:A:TYR:HB3	1:280:A:GLU:HB2	16	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD11	10	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD12	10	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD13	10	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD21	10	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD22	10	0.18
(1,408)	1:277:A:LEU:H	1:277:A:LEU:HD23	10	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD11	11	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD12	11	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD13	11	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD21	11	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD22	11	0.18
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD23	11	0.18
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB2	9	0.18
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB3	9	0.18
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB2	9	0.18
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB3	9	0.18
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB2	9	0.18
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB3	9	0.18
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	6	0.18
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	9	0.18
(1,348)	1:272:A:THR:HB	1:273:A:THR:H	15	0.18
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	5	0.18
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	5	0.18
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	5	0.18
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	13	0.18
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	4	0.18
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	4	0.18
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	4	0.18
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	4	0.18
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	4	0.18
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	4	0.18
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD2	8	0.18
(1,156)	1:247:A:ALA:H	1:248:A:ARG:HD3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	9	0.18
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	9	0.18
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	9	0.18
(1,148)	1:246:A:LYS:HB2	1:247:A:ALA:H	4	0.18
(1,148)	1:246:A:LYS:HB3	1:247:A:ALA:H	4	0.18
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	5	0.18
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	5	0.18
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	6	0.18
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	6	0.18
(1,38)	1:228:A:MET:HA	1:229:A:LYS:H	6	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG11	7	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG12	7	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG13	7	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG21	7	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG22	7	0.18
(1,8)	1:224:A:LYS:HA	1:225:A:VAL:HG23	7	0.18
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	11	0.17
(1,1985)	1:310:A:PHE:H	1:476:A:PHE:HZ	6	0.17
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	13	0.17
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	13	0.17
(1,1977)	1:473:A:LYS:HD2	1:475:A:VAL:HB	20	0.17
(1,1977)	1:473:A:LYS:HD3	1:475:A:VAL:HB	20	0.17
(1,1933)	1:470:A:LEU:HD11	1:474:A:LEU:H	17	0.17
(1,1933)	1:470:A:LEU:HD12	1:474:A:LEU:H	17	0.17
(1,1933)	1:470:A:LEU:HD13	1:474:A:LEU:H	17	0.17
(1,1888)	1:224:A:LYS:HA	1:473:A:LYS:H	13	0.17
(1,1854)	1:469:A:THR:HG21	1:470:A:LEU:H	15	0.17
(1,1854)	1:469:A:THR:HG22	1:470:A:LEU:H	15	0.17
(1,1854)	1:469:A:THR:HG23	1:470:A:LEU:H	15	0.17
(1,1852)	1:440:A:LEU:HD11	1:470:A:LEU:HD21	7	0.17
(1,1852)	1:440:A:LEU:HD11	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD11	1:470:A:LEU:HD23	7	0.17
(1,1852)	1:440:A:LEU:HD12	1:470:A:LEU:HD21	7	0.17
(1,1852)	1:440:A:LEU:HD12	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD12	1:470:A:LEU:HD23	7	0.17
(1,1852)	1:440:A:LEU:HD13	1:470:A:LEU:HD21	7	0.17
(1,1852)	1:440:A:LEU:HD13	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD13	1:470:A:LEU:HD23	7	0.17
(1,1852)	1:440:A:LEU:HD21	1:470:A:LEU:HD21	7	0.17
(1,1852)	1:440:A:LEU:HD21	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD21	1:470:A:LEU:HD23	7	0.17
(1,1852)	1:440:A:LEU:HD22	1:470:A:LEU:HD21	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1852)	1:440:A:LEU:HD22	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD22	1:470:A:LEU:HD23	7	0.17
(1,1852)	1:440:A:LEU:HD23	1:470:A:LEU:HD21	7	0.17
(1,1852)	1:440:A:LEU:HD23	1:470:A:LEU:HD22	7	0.17
(1,1852)	1:440:A:LEU:HD23	1:470:A:LEU:HD23	7	0.17
(1,1835)	1:398:A:ASP:H	1:470:A:LEU:HG	8	0.17
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	1	0.17
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	1	0.17
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	1	0.17
(1,1821)	1:398:A:ASP:H	1:469:A:THR:HB	10	0.17
(1,1820)	1:397:A:ALA:HB1	1:469:A:THR:HB	20	0.17
(1,1820)	1:397:A:ALA:HB2	1:469:A:THR:HB	20	0.17
(1,1820)	1:397:A:ALA:HB3	1:469:A:THR:HB	20	0.17
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	14	0.17
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	14	0.17
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	14	0.17
(1,1816)	1:467:A:THR:HA	1:468:A:PHE:H	18	0.17
(1,1719)	1:439:A:ILE:HG21	1:441:A:THR:H	6	0.17
(1,1719)	1:439:A:ILE:HG22	1:441:A:THR:H	6	0.17
(1,1719)	1:439:A:ILE:HG23	1:441:A:THR:H	6	0.17
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	3	0.17
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	3	0.17
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	3	0.17
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	3	0.17
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	12	0.17
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	12	0.17
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	15	0.17
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	15	0.17
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	16	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD11	14	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD12	14	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD13	14	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD21	14	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD22	14	0.17
(1,1553)	1:422:A:ILE:HD11	1:425:A:LEU:HD23	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD11	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD12	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD13	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD21	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD22	14	0.17
(1,1553)	1:422:A:ILE:HD12	1:425:A:LEU:HD23	14	0.17
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD11	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD12	14	0.17
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD13	14	0.17
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD21	14	0.17
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD22	14	0.17
(1,1553)	1:422:A:ILE:HD13	1:425:A:LEU:HD23	14	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD11	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD12	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD13	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD21	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD22	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD23	3	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD11	16	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD12	16	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD13	16	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD21	16	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD22	16	0.17
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD23	16	0.17
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB2	7	0.17
(1,1543)	1:424:A:SER:H	1:424:A:SER:HB3	7	0.17
(1,1534)	1:422:A:ILE:HB	1:423:A:GLN:H	14	0.17
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	11	0.17
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	11	0.17
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	11	0.17
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	11	0.17
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	11	0.17
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	11	0.17
(1,1493)	1:400:A:LEU:HD11	1:402:A:GLY:H	18	0.17
(1,1493)	1:400:A:LEU:HD12	1:402:A:GLY:H	18	0.17
(1,1493)	1:400:A:LEU:HD13	1:402:A:GLY:H	18	0.17
(1,1493)	1:400:A:LEU:HD21	1:402:A:GLY:H	18	0.17
(1,1493)	1:400:A:LEU:HD22	1:402:A:GLY:H	18	0.17
(1,1493)	1:400:A:LEU:HD23	1:402:A:GLY:H	18	0.17
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD11	1:401:A:LEU:HB3	17	0.17
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD12	1:401:A:LEU:HB3	17	0.17
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD13	1:401:A:LEU:HB3	17	0.17
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD21	1:401:A:LEU:HB3	17	0.17
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD22	1:401:A:LEU:HB3	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB2	17	0.17
(1,1485)	1:400:A:LEU:HD23	1:401:A:LEU:HB3	17	0.17
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG21	7	0.17
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG22	7	0.17
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG23	7	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG21	7	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG22	7	0.17
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG23	7	0.17
(1,1411)	1:389:A:GLN:HE21	1:390:A:THR:HB	1	0.17
(1,1411)	1:389:A:GLN:HE22	1:390:A:THR:HB	1	0.17
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	4	0.17
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	4	0.17
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	4	0.17
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	4	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD11	20	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD12	20	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD13	20	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD21	20	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD22	20	0.17
(1,1376)	1:380:A:TYR:HB2	1:381:A:LEU:HD23	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD11	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD12	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD13	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD21	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD22	20	0.17
(1,1376)	1:380:A:TYR:HB3	1:381:A:LEU:HD23	20	0.17
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	11	0.17
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	16	0.17
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	3	0.17
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	3	0.17
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	3	0.17
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	3	0.17
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB2	13	0.17
(1,1361)	1:376:A:GLU:HB2	1:381:A:LEU:HB3	13	0.17
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB2	13	0.17
(1,1361)	1:376:A:GLU:HB3	1:381:A:LEU:HB3	13	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	10	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	10	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	10	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	10	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	10	0.17
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	6	0.17
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	6	0.17
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	6	0.17
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	6	0.17
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	6	0.17
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	20	0.17
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	20	0.17
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	20	0.17
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	20	0.17
(1,1338)	1:373:A:THR:HB	1:380:A:TYR:HA	13	0.17
(1,1320)	1:248:A:ARG:HD2	1:376:A:GLU:HA	3	0.17
(1,1320)	1:248:A:ARG:HD3	1:376:A:GLU:HA	3	0.17
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	11	0.17
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	11	0.17
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	16	0.17
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	16	0.17
(1,1267)	1:360:A:ALA:HB1	1:361:A:GLN:HA	12	0.17
(1,1267)	1:360:A:ALA:HB2	1:361:A:GLN:HA	12	0.17
(1,1267)	1:360:A:ALA:HB3	1:361:A:GLN:HA	12	0.17
(1,1255)	1:357:A:ILE:HG21	1:359:A:ALA:HA	18	0.17
(1,1255)	1:357:A:ILE:HG22	1:359:A:ALA:HA	18	0.17
(1,1255)	1:357:A:ILE:HG23	1:359:A:ALA:HA	18	0.17
(1,1236)	1:314:A:ILE:H	1:356:A:PHE:H	4	0.17
(1,1233)	1:312:A:CYS:H	1:356:A:PHE:H	4	0.17
(1,1225)	1:354:A:VAL:HB	1:355:A:PHE:H	10	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG11	11	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG12	11	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG13	11	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG21	11	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG22	11	0.17
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG23	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG11	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG12	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG13	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG21	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG22	11	0.17
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG23	11	0.17
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	5	0.17
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	5	0.17
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	5	0.17
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	5	0.17
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	5	0.17
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	6	0.17
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	13	0.17
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	6	0.17
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB2	11	0.17
(1,1162)	1:345:A:CYS:H	1:346:A:PRO:HB3	11	0.17
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	18	0.17
(1,1129)	1:341:A:THR:HG21	1:344:A:LYS:HG2	2	0.17
(1,1129)	1:341:A:THR:HG22	1:344:A:LYS:HG2	2	0.17
(1,1129)	1:341:A:THR:HG23	1:344:A:LYS:HG2	2	0.17
(1,1110)	1:341:A:THR:HB	1:343:A:LEU:HG	15	0.17
(1,1085)	1:337:A:THR:H	1:339:A:GLN:H	11	0.17
(1,1079)	1:337:A:THR:HG21	1:338:A:SER:H	10	0.17
(1,1079)	1:337:A:THR:HG22	1:338:A:SER:H	10	0.17
(1,1079)	1:337:A:THR:HG23	1:338:A:SER:H	10	0.17
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG21	16	0.17
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG22	16	0.17
(1,1065)	1:335:A:GLU:H	1:337:A:THR:HG23	16	0.17
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	6	0.17
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	6	0.17
(1,1017)	1:333:A:ILE:HA	1:335:A:GLU:H	11	0.17
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB2	18	0.17
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB3	18	0.17
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB2	18	0.17
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB3	18	0.17
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB2	18	0.17
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB3	18	0.17
(1,910)	1:322:A:ILE:HA	1:323:A:ILE:H	16	0.17
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG12	12	0.17
(1,909)	1:322:A:ILE:H	1:322:A:ILE:HG13	12	0.17
(1,898)	1:320:A:LYS:HB2	1:322:A:ILE:H	10	0.17
(1,898)	1:320:A:LYS:HB3	1:322:A:ILE:H	10	0.17
(1,894)	1:319:A:ASP:HA	1:322:A:ILE:HG12	6	0.17
(1,894)	1:319:A:ASP:HA	1:322:A:ILE:HG13	6	0.17
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	20	0.17
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	20	0.17
(1,803)	1:309:A:CYS:HB2	1:310:A:PHE:H	13	0.17
(1,803)	1:309:A:CYS:HB3	1:310:A:PHE:H	13	0.17
(1,801)	1:309:A:CYS:HB2	1:310:A:PHE:H	11	0.17
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	13	0.17
(1,767)	1:302:A:MET:HG2	1:303:A:ASP:H	2	0.17
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:298:A:ILE:H	1:300:A:GLN:H	18	0.17
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	6	0.17
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	6	0.17
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	6	0.17
(1,682)	1:298:A:ILE:H	1:298:A:ILE:HD11	11	0.17
(1,682)	1:298:A:ILE:H	1:298:A:ILE:HD12	11	0.17
(1,682)	1:298:A:ILE:H	1:298:A:ILE:HD13	11	0.17
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD11	10	0.17
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD12	10	0.17
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD13	10	0.17
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD11	10	0.17
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD12	10	0.17
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD13	10	0.17
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD11	10	0.17
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD12	10	0.17
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD13	10	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	1	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	1	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	1	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	4	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	4	0.17
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	4	0.17
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD2	6	0.17
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD3	6	0.17
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	14	0.17
(1,505)	1:239:A:ILE:HA	1:285:A:ASP:HA	18	0.17
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG12	18	0.17
(1,446)	1:236:A:CYS:H	1:281:A:ILE:HG13	18	0.17
(1,434)	1:235:A:TYR:HD1	1:280:A:GLU:H	3	0.17
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD11	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD12	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD13	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD21	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD22	15	0.17
(1,315)	1:267:A:ALA:HA	1:270:A:LEU:HD23	15	0.17
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	2	0.17
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	2	0.17
(1,259)	1:256:A:SER:H	1:257:A:ILE:HG21	13	0.17
(1,259)	1:256:A:SER:H	1:257:A:ILE:HG22	13	0.17
(1,259)	1:256:A:SER:H	1:257:A:ILE:HG23	13	0.17
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG21	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG22	6	0.17
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG23	6	0.17
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG21	6	0.17
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG22	6	0.17
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG23	6	0.17
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	17	0.17
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	10	0.17
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	10	0.17
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	10	0.17
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG11	1:253:A:LYS:HD3	12	0.17
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG12	1:253:A:LYS:HD3	12	0.17
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG13	1:253:A:LYS:HD3	12	0.17
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG21	1:253:A:LYS:HD3	12	0.17
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG22	1:253:A:LYS:HD3	12	0.17
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD2	12	0.17
(1,204)	1:251:A:VAL:HG23	1:253:A:LYS:HD3	12	0.17
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	17	0.17
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	17	0.17
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	17	0.17
(1,118)	1:241:A:ASN:HA	1:243:A:ASN:H	9	0.17
(1,90)	1:237:A:LEU:HB2	1:238:A:ILE:H	3	0.17
(1,90)	1:237:A:LEU:HB3	1:238:A:ILE:H	3	0.17
(1,79)	1:235:A:TYR:H	1:236:A:CYS:H	8	0.17
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	17	0.17
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	17	0.17
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	5	0.17
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	5	0.17
(1,52)	1:230:A:SER:H	1:231:A:LYS:H	4	0.17
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	1	0.17
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	1	0.17
(1,3)	1:224:A:LYS:HA	1:224:A:LYS:HE2	15	0.17
(1,3)	1:224:A:LYS:HA	1:224:A:LYS:HE3	15	0.17
(1,1985)	1:310:A:PHE:H	1:476:A:PHE:HZ	20	0.16
(1,1952)	1:225:A:VAL:HG11	1:475:A:VAL:H	19	0.16
(1,1952)	1:225:A:VAL:HG12	1:475:A:VAL:H	19	0.16
(1,1952)	1:225:A:VAL:HG13	1:475:A:VAL:H	19	0.16
(1,1952)	1:225:A:VAL:HG21	1:475:A:VAL:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1952)	1:225:A:VAL:HG22	1:475:A:VAL:H	19	0.16
(1,1952)	1:225:A:VAL:HG23	1:475:A:VAL:H	19	0.16
(1,1888)	1:224:A:LYS:HA	1:473:A:LYS:H	20	0.16
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	13	0.16
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	18	0.16
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	18	0.16
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	18	0.16
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	16	0.16
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG21	5	0.16
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG22	5	0.16
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG23	5	0.16
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG21	5	0.16
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG22	5	0.16
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG23	5	0.16
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	5	0.16
(1,1675)	1:435:A:ARG:HG2	1:437:A:ASP:H	7	0.16
(1,1675)	1:435:A:ARG:HG3	1:437:A:ASP:H	7	0.16
(1,1671)	1:435:A:ARG:HG2	1:436:A:GLY:H	3	0.16
(1,1671)	1:435:A:ARG:HG3	1:436:A:GLY:H	3	0.16
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	12	0.16
(1,1587)	1:427:A:GLN:HB2	1:428:A:SER:H	9	0.16
(1,1587)	1:427:A:GLN:HB3	1:428:A:SER:H	9	0.16
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	9	0.16
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	9	0.16
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	9	0.16
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	9	0.16
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	9	0.16
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	9	0.16
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	12	0.16
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	12	0.16
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	12	0.16
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	12	0.16
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	12	0.16
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	12	0.16
(1,1489)	1:356:A:PHE:HA	1:402:A:GLY:H	11	0.16
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG21	15	0.16
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG22	15	0.16
(1,1424)	1:393:A:ILE:H	1:393:A:ILE:HG23	15	0.16
(1,1420)	1:333:A:ILE:HG21	1:392:A:TYR:HE1	8	0.16
(1,1420)	1:333:A:ILE:HG22	1:392:A:TYR:HE1	8	0.16
(1,1420)	1:333:A:ILE:HG23	1:392:A:TYR:HE1	8	0.16
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	5	0.16
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB2	5	0.16
(1,1399)	1:384:A:ASP:HB2	1:385:A:LEU:HB3	5	0.16
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB2	5	0.16
(1,1399)	1:384:A:ASP:HB3	1:385:A:LEU:HB3	5	0.16
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	5	0.16
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	5	0.16
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	5	0.16
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	5	0.16
(1,1373)	1:380:A:TYR:HA	1:381:A:LEU:HG	11	0.16
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	1	0.16
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	1	0.16
(1,1356)	1:373:A:THR:HB	1:381:A:LEU:HG	8	0.16
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	1	0.16
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	4	0.16
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	4	0.16
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	4	0.16
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	4	0.16
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	17	0.16
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	17	0.16
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	17	0.16
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	17	0.16
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	1	0.16
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	1	0.16
(1,1330)	1:377:A:GLU:HB2	1:378:A:GLN:HA	6	0.16
(1,1330)	1:377:A:GLU:HB3	1:378:A:GLN:HA	6	0.16
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	6	0.16
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	6	0.16
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	12	0.16
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	12	0.16
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	12	0.16
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	12	0.16
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	12	0.16
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	12	0.16
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	16	0.16
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	16	0.16
(1,1250)	1:357:A:ILE:HA	1:358:A:GLN:H	17	0.16
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG11	10	0.16
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG12	10	0.16
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG13	10	0.16
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG21	10	0.16
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG22	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:353:A:LYS:H	1:354:A:VAL:HG23	10	0.16
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	8	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	4	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	4	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	4	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB1	15	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB2	15	0.16
(1,1185)	1:348:A:LEU:H	1:349:A:ALA:HB3	15	0.16
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	14	0.16
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	14	0.16
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	17	0.16
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	17	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	5	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	5	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	5	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	5	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	5	0.16
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	5	0.16
(1,1092)	1:339:A:GLN:H	1:340:A:PHE:HA	11	0.16
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG21	4	0.16
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG22	4	0.16
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG23	4	0.16
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG21	4	0.16
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG22	4	0.16
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG23	4	0.16
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG21	4	0.16
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG22	4	0.16
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG23	4	0.16
(1,1058)	1:296:A:LEU:HD11	1:337:A:THR:HB	11	0.16
(1,1058)	1:296:A:LEU:HD12	1:337:A:THR:HB	11	0.16
(1,1058)	1:296:A:LEU:HD13	1:337:A:THR:HB	11	0.16
(1,1058)	1:296:A:LEU:HD21	1:337:A:THR:HB	11	0.16
(1,1058)	1:296:A:LEU:HD22	1:337:A:THR:HB	11	0.16
(1,1058)	1:296:A:LEU:HD23	1:337:A:THR:HB	11	0.16
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB2	4	0.16
(1,1025)	1:293:A:TYR:HD1	1:336:A:LEU:HB3	4	0.16
(1,1022)	1:334:A:TYR:HB2	1:335:A:GLU:H	6	0.16
(1,1011)	1:333:A:ILE:HG21	1:334:A:TYR:HE1	18	0.16
(1,1011)	1:333:A:ILE:HG22	1:334:A:TYR:HE1	18	0.16
(1,1011)	1:333:A:ILE:HG23	1:334:A:TYR:HE1	18	0.16
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	2	0.16
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:288:A:THR:HG21	1:326:A:THR:H	8	0.16
(1,935)	1:288:A:THR:HG22	1:326:A:THR:H	8	0.16
(1,935)	1:288:A:THR:HG23	1:326:A:THR:H	8	0.16
(1,930)	1:324:A:TYR:HD1	1:325:A:GLY:H	19	0.16
(1,914)	1:322:A:ILE:H	1:323:A:ILE:H	5	0.16
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	4	0.16
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	4	0.16
(1,898)	1:320:A:LYS:HB2	1:322:A:ILE:H	18	0.16
(1,898)	1:320:A:LYS:HB3	1:322:A:ILE:H	18	0.16
(1,801)	1:309:A:CYS:HB2	1:310:A:PHE:H	19	0.16
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	16	0.16
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	10	0.16
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB2	11	0.16
(1,768)	1:302:A:MET:HB2	1:303:A:ASP:HB3	11	0.16
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	2	0.16
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	2	0.16
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	2	0.16
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	6	0.16
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	17	0.16
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	12	0.16
(1,706)	1:298:A:ILE:HD11	1:299:A:TYR:HE1	6	0.16
(1,706)	1:298:A:ILE:HD12	1:299:A:TYR:HE1	6	0.16
(1,706)	1:298:A:ILE:HD13	1:299:A:TYR:HE1	6	0.16
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	8	0.16
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	8	0.16
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	8	0.16
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	8	0.16
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG12	20	0.16
(1,677)	1:297:A:LYS:HD2	1:298:A:ILE:HG13	20	0.16
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG12	20	0.16
(1,677)	1:297:A:LYS:HD3	1:298:A:ILE:HG13	20	0.16
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	13	0.16
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	13	0.16
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	13	0.16
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD2	3	0.16
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD3	3	0.16
(1,626)	1:292:A:ILE:HB	1:295:A:ILE:HD11	6	0.16
(1,626)	1:292:A:ILE:HB	1:295:A:ILE:HD12	6	0.16
(1,626)	1:292:A:ILE:HB	1:295:A:ILE:HD13	6	0.16
(1,625)	1:292:A:ILE:HG12	1:295:A:ILE:HG12	11	0.16
(1,625)	1:292:A:ILE:HG12	1:295:A:ILE:HG13	11	0.16
(1,625)	1:292:A:ILE:HG13	1:295:A:ILE:HG12	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:292:A:ILE:HG13	1:295:A:ILE:HG13	11	0.16
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD11	10	0.16
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD12	10	0.16
(1,624)	1:292:A:ILE:HD11	1:295:A:ILE:HD13	10	0.16
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD11	10	0.16
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD12	10	0.16
(1,624)	1:292:A:ILE:HD12	1:295:A:ILE:HD13	10	0.16
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD11	10	0.16
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD12	10	0.16
(1,624)	1:292:A:ILE:HD13	1:295:A:ILE:HD13	10	0.16
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	18	0.16
(1,594)	1:290:A:GLU:HA	1:293:A:TYR:H	6	0.16
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG2	1	0.16
(1,558)	1:291:A:GLN:H	1:291:A:GLN:HG3	1	0.16
(1,491)	1:238:A:ILE:HD11	1:283:A:PRO:HA	6	0.16
(1,491)	1:238:A:ILE:HD12	1:283:A:PRO:HA	6	0.16
(1,491)	1:238:A:ILE:HD13	1:283:A:PRO:HA	6	0.16
(1,422)	1:275:A:GLU:HA	1:279:A:PHE:H	17	0.16
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB2	2	0.16
(1,421)	1:236:A:CYS:H	1:279:A:PHE:HB3	2	0.16
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	11	0.16
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	19	0.16
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB2	3	0.16
(1,386)	1:272:A:THR:HG21	1:276:A:GLU:HB3	3	0.16
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB2	3	0.16
(1,386)	1:272:A:THR:HG22	1:276:A:GLU:HB3	3	0.16
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB2	3	0.16
(1,386)	1:272:A:THR:HG23	1:276:A:GLU:HB3	3	0.16
(1,377)	1:273:A:THR:HB	1:275:A:GLU:H	17	0.16
(1,346)	1:271:A:THR:H	1:273:A:THR:H	3	0.16
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	10	0.16
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	10	0.16
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	10	0.16
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	13	0.16
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	19	0.16
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	19	0.16
(1,276)	1:258:A:ARG:H	1:259:A:ASP:HA	15	0.16
(1,268)	1:257:A:ILE:HB	1:258:A:ARG:H	12	0.16
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	19	0.16
(1,227)	1:253:A:LYS:HE2	1:254:A:LEU:HG	12	0.16
(1,227)	1:253:A:LYS:HE3	1:254:A:LEU:HG	12	0.16
(1,217)	1:251:A:VAL:HG21	1:254:A:LEU:HG	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:251:A:VAL:HG22	1:254:A:LEU:HG	14	0.16
(1,217)	1:251:A:VAL:HG23	1:254:A:LEU:HG	14	0.16
(1,210)	1:247:A:ALA:HA	1:254:A:LEU:HG	11	0.16
(1,176)	1:249:A:GLU:HB2	1:250:A:LYS:HA	11	0.16
(1,176)	1:249:A:GLU:HB3	1:250:A:LYS:HA	11	0.16
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	19	0.16
(1,161)	1:247:A:ALA:HB1	1:249:A:GLU:H	12	0.16
(1,161)	1:247:A:ALA:HB2	1:249:A:GLU:H	12	0.16
(1,161)	1:247:A:ALA:HB3	1:249:A:GLU:H	12	0.16
(1,155)	1:247:A:ALA:HB1	1:248:A:ARG:HA	14	0.16
(1,155)	1:247:A:ALA:HB2	1:248:A:ARG:HA	14	0.16
(1,155)	1:247:A:ALA:HB3	1:248:A:ARG:HA	14	0.16
(1,87)	1:237:A:LEU:HD21	1:238:A:ILE:H	12	0.16
(1,87)	1:237:A:LEU:HD22	1:238:A:ILE:H	12	0.16
(1,87)	1:237:A:LEU:HD23	1:238:A:ILE:H	12	0.16
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	6	0.16
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	19	0.16
(1,71)	1:232:A:PRO:HA	1:234:A:GLY:H	6	0.16
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	14	0.16
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	14	0.16
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	8	0.16
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	8	0.16
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	6	0.15
(1,1999)	1:475:A:VAL:HB	1:476:A:PHE:H	16	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG11	13	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG12	13	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG13	13	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG21	13	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG22	13	0.15
(1,1975)	1:473:A:LYS:HA	1:475:A:VAL:HG23	13	0.15
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	11	0.15
(1,1835)	1:398:A:ASP:H	1:470:A:LEU:HG	10	0.15
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	6	0.15
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	6	0.15
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	6	0.15
(1,1809)	1:400:A:LEU:HD11	1:468:A:PHE:HA	18	0.15
(1,1809)	1:400:A:LEU:HD12	1:468:A:PHE:HA	18	0.15
(1,1809)	1:400:A:LEU:HD13	1:468:A:PHE:HA	18	0.15
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG11	4	0.15
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG12	4	0.15
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG13	4	0.15
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG22	4	0.15
(1,1791)	1:426:A:CYS:H	1:446:A:VAL:HG23	4	0.15
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	17	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	11	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	11	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	11	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	11	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	11	0.15
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	11	0.15
(1,1748)	1:356:A:PHE:HE1	1:443:A:LEU:H	17	0.15
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD11	9	0.15
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD12	9	0.15
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD13	9	0.15
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD11	17	0.15
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD12	17	0.15
(1,1731)	1:437:A:ASP:H	1:442:A:ILE:HD13	17	0.15
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG21	11	0.15
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG22	11	0.15
(1,1729)	1:433:A:CYS:HA	1:442:A:ILE:HG23	11	0.15
(1,1721)	1:440:A:LEU:HG	1:441:A:THR:H	15	0.15
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB2	19	0.15
(1,1703)	1:438:A:ASP:HA	1:440:A:LEU:HB3	19	0.15
(1,1676)	1:435:A:ARG:HB2	1:437:A:ASP:H	15	0.15
(1,1676)	1:435:A:ARG:HB3	1:437:A:ASP:H	15	0.15
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	17	0.15
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	17	0.15
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	18	0.15
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	18	0.15
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	11	0.15
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	11	0.15
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	11	0.15
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	13	0.15
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	13	0.15
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	13	0.15
(1,1605)	1:273:A:THR:HG21	1:430:A:ARG:HG3	14	0.15
(1,1605)	1:273:A:THR:HG22	1:430:A:ARG:HG3	14	0.15
(1,1605)	1:273:A:THR:HG23	1:430:A:ARG:HG3	14	0.15
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG2	18	0.15
(1,1523)	1:416:A:ALA:HB1	1:417:A:GLU:HG3	18	0.15
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG2	18	0.15
(1,1523)	1:416:A:ALA:HB2	1:417:A:GLU:HG3	18	0.15
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	1:416:A:ALA:HB3	1:417:A:GLU:HG3	18	0.15
(1,1478)	1:355:A:PHE:H	1:401:A:LEU:HA	8	0.15
(1,1409)	1:389:A:GLN:HG2	1:390:A:THR:HA	2	0.15
(1,1409)	1:389:A:GLN:HG3	1:390:A:THR:HA	2	0.15
(1,1409)	1:389:A:GLN:HG2	1:390:A:THR:HA	16	0.15
(1,1409)	1:389:A:GLN:HG3	1:390:A:THR:HA	16	0.15
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	12	0.15
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	12	0.15
(1,1370)	1:380:A:TYR:HB2	1:381:A:LEU:HG	14	0.15
(1,1370)	1:380:A:TYR:HB3	1:381:A:LEU:HG	14	0.15
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	5	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	15	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	15	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	15	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	15	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	15	0.15
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	15	0.15
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB2	17	0.15
(1,1358)	1:373:A:THR:HG21	1:381:A:LEU:HB3	17	0.15
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB2	17	0.15
(1,1358)	1:373:A:THR:HG22	1:381:A:LEU:HB3	17	0.15
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB2	17	0.15
(1,1358)	1:373:A:THR:HG23	1:381:A:LEU:HB3	17	0.15
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB2	13	0.15
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB3	13	0.15
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB2	13	0.15
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB3	13	0.15
(1,1347)	1:380:A:TYR:H	1:380:A:TYR:HD1	12	0.15
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG2	8	0.15
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG3	8	0.15
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	20	0.15
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	20	0.15
(1,1239)	1:355:A:PHE:H	1:356:A:PHE:H	11	0.15
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	14	0.15
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	16	0.15
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	16	0.15
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	16	0.15
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	16	0.15
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	16	0.15
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	1	0.15
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	7	0.15
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	9	0.15
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	2	0.15
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	2	0.15
(1,1147)	1:341:A:THR:HG21	1:345:A:CYS:H	16	0.15
(1,1147)	1:341:A:THR:HG22	1:345:A:CYS:H	16	0.15
(1,1147)	1:341:A:THR:HG23	1:345:A:CYS:H	16	0.15
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE2	7	0.15
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE3	7	0.15
(1,1125)	1:341:A:THR:HA	1:344:A:LYS:H	15	0.15
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	9	0.15
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	9	0.15
(1,1098)	1:340:A:PHE:H	1:341:A:THR:HA	11	0.15
(1,1098)	1:340:A:PHE:H	1:341:A:THR:HA	17	0.15
(1,1092)	1:339:A:GLN:H	1:340:A:PHE:HA	6	0.15
(1,1079)	1:337:A:THR:HG21	1:338:A:SER:H	17	0.15
(1,1079)	1:337:A:THR:HG22	1:338:A:SER:H	17	0.15
(1,1079)	1:337:A:THR:HG23	1:338:A:SER:H	17	0.15
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG21	20	0.15
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG22	20	0.15
(1,1062)	1:333:A:ILE:HG21	1:337:A:THR:HG23	20	0.15
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG21	20	0.15
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG22	20	0.15
(1,1062)	1:333:A:ILE:HG22	1:337:A:THR:HG23	20	0.15
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG21	20	0.15
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG22	20	0.15
(1,1062)	1:333:A:ILE:HG23	1:337:A:THR:HG23	20	0.15
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	14	0.15
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	14	0.15
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	14	0.15
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	3	0.15
(1,1008)	1:333:A:ILE:HD11	1:334:A:TYR:H	16	0.15
(1,1008)	1:333:A:ILE:HD12	1:334:A:TYR:H	16	0.15
(1,1008)	1:333:A:ILE:HD13	1:334:A:TYR:H	16	0.15
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	14	0.15
(1,970)	1:328:A:GLY:H	1:329:A:GLN:H	11	0.15
(1,964)	1:289:A:VAL:HG11	1:329:A:GLN:H	5	0.15
(1,964)	1:289:A:VAL:HG12	1:329:A:GLN:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:289:A:VAL:HG13	1:329:A:GLN:H	5	0.15
(1,964)	1:289:A:VAL:HG21	1:329:A:GLN:H	5	0.15
(1,964)	1:289:A:VAL:HG22	1:329:A:GLN:H	5	0.15
(1,964)	1:289:A:VAL:HG23	1:329:A:GLN:H	5	0.15
(1,955)	1:250:A:LYS:HG2	1:328:A:GLY:H	1	0.15
(1,955)	1:250:A:LYS:HG3	1:328:A:GLY:H	1	0.15
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA2	12	0.15
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA3	12	0.15
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA2	12	0.15
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA3	12	0.15
(1,946)	1:288:A:THR:HG21	1:327:A:ASP:H	3	0.15
(1,946)	1:288:A:THR:HG22	1:327:A:ASP:H	3	0.15
(1,946)	1:288:A:THR:HG23	1:327:A:ASP:H	3	0.15
(1,931)	1:324:A:TYR:HB2	1:325:A:GLY:H	19	0.15
(1,914)	1:322:A:ILE:H	1:323:A:ILE:H	1	0.15
(1,914)	1:322:A:ILE:H	1:323:A:ILE:H	20	0.15
(1,912)	1:322:A:ILE:HB	1:323:A:ILE:H	3	0.15
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD2	15	0.15
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD3	15	0.15
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	18	0.15
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	18	0.15
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	11	0.15
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	11	0.15
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	12	0.15
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	12	0.15
(1,855)	1:239:A:ILE:HG21	1:315:A:LEU:H	7	0.15
(1,855)	1:239:A:ILE:HG22	1:315:A:LEU:H	7	0.15
(1,855)	1:239:A:ILE:HG23	1:315:A:LEU:H	7	0.15
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	11	0.15
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	11	0.15
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	11	0.15
(1,803)	1:309:A:CYS:HB2	1:310:A:PHE:H	3	0.15
(1,803)	1:309:A:CYS:HB3	1:310:A:PHE:H	3	0.15
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	5	0.15
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	5	0.15
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE1	12	0.15
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE2	12	0.15
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE3	12	0.15
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE1	12	0.15
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE2	12	0.15
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE3	12	0.15
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE1	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE2	14	0.15
(1,783)	1:235:A:TYR:HD1	1:307:A:MET:HE3	14	0.15
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB2	15	0.15
(1,782)	1:305:A:SER:H	1:306:A:ASN:HB3	15	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD11	1	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD12	1	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD13	1	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD21	1	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD22	1	0.15
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD23	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD11	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD12	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD13	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD21	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD22	1	0.15
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD23	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD11	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD12	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD13	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD21	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD22	1	0.15
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD23	1	0.15
(1,708)	1:299:A:TYR:H	1:299:A:TYR:HD1	1	0.15
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	10	0.15
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	16	0.15
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	16	0.15
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	16	0.15
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	7	0.15
(1,550)	1:287:A:CYS:HB2	1:291:A:GLN:H	11	0.15
(1,550)	1:287:A:CYS:HB3	1:291:A:GLN:H	11	0.15
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	3	0.15
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	3	0.15
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	3	0.15
(1,523)	1:239:A:ILE:HG21	1:287:A:CYS:H	11	0.15
(1,523)	1:239:A:ILE:HG22	1:287:A:CYS:H	11	0.15
(1,523)	1:239:A:ILE:HG23	1:287:A:CYS:H	11	0.15
(1,508)	1:240:A:ASN:HB2	1:285:A:ASP:H	18	0.15
(1,508)	1:240:A:ASN:HB3	1:285:A:ASP:H	18	0.15
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB2	3	0.15
(1,495)	1:238:A:ILE:H	1:284:A:HIS:HB3	3	0.15
(1,479)	1:238:A:ILE:HB	1:282:A:LYS:H	19	0.15
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD11	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD12	9	0.15
(1,462)	1:278:A:HIS:H	1:281:A:ILE:HD13	9	0.15
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG21	2	0.15
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG22	2	0.15
(1,451)	1:271:A:THR:HB	1:281:A:ILE:HG23	2	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD11	12	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD12	12	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD13	12	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD21	12	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD22	12	0.15
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD23	12	0.15
(1,314)	1:267:A:ALA:HA	1:270:A:LEU:HG	1	0.15
(1,281)	1:264:A:HIS:HD2	1:265:A:LEU:HG	13	0.15
(1,270)	1:257:A:ILE:HG12	1:258:A:ARG:H	10	0.15
(1,270)	1:257:A:ILE:HG13	1:258:A:ARG:H	10	0.15
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD11	15	0.15
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD12	15	0.15
(1,256)	1:255:A:HIS:H	1:257:A:ILE:HD13	15	0.15
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG21	20	0.15
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG22	20	0.15
(1,254)	1:255:A:HIS:HA	1:257:A:ILE:HG23	20	0.15
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	6	0.15
(1,227)	1:253:A:LYS:HE2	1:254:A:LEU:HG	1	0.15
(1,227)	1:253:A:LYS:HE3	1:254:A:LEU:HG	1	0.15
(1,221)	1:251:A:VAL:HG11	1:254:A:LEU:H	19	0.15
(1,221)	1:251:A:VAL:HG12	1:254:A:LEU:H	19	0.15
(1,221)	1:251:A:VAL:HG13	1:254:A:LEU:H	19	0.15
(1,221)	1:251:A:VAL:HG21	1:254:A:LEU:H	19	0.15
(1,221)	1:251:A:VAL:HG22	1:254:A:LEU:H	19	0.15
(1,221)	1:251:A:VAL:HG23	1:254:A:LEU:H	19	0.15
(1,219)	1:251:A:VAL:HG11	1:254:A:LEU:HG	13	0.15
(1,219)	1:251:A:VAL:HG12	1:254:A:LEU:HG	13	0.15
(1,219)	1:251:A:VAL:HG13	1:254:A:LEU:HG	13	0.15
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	16	0.15
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	14	0.15
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	14	0.15
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	14	0.15
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	14	0.15
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	14	0.15
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	14	0.15
(1,161)	1:247:A:ALA:HB1	1:249:A:GLU:H	2	0.15
(1,161)	1:247:A:ALA:HB2	1:249:A:GLU:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:247:A:ALA:HB3	1:249:A:GLU:H	2	0.15
(1,148)	1:246:A:LYS:HB2	1:247:A:ALA:H	12	0.15
(1,148)	1:246:A:LYS:HB3	1:247:A:ALA:H	12	0.15
(1,127)	1:244:A:PHE:HA	1:245:A:ALA:H	4	0.15
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	16	0.15
(1,70)	1:232:A:PRO:HG2	1:233:A:ARG:HA	2	0.15
(1,70)	1:232:A:PRO:HG3	1:233:A:ARG:HA	2	0.15
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	10	0.15
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	10	0.15
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG2	7	0.15
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG3	7	0.15
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG2	7	0.15
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG3	7	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG11	13	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG12	13	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG13	13	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG21	13	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG22	13	0.15
(1,9)	1:224:A:LYS:HG2	1:225:A:VAL:HG23	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG11	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG12	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG13	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG21	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG22	13	0.15
(1,9)	1:224:A:LYS:HG3	1:225:A:VAL:HG23	13	0.15
(1,6)	1:224:A:LYS:HB2	1:225:A:VAL:H	20	0.15
(1,5)	1:224:A:LYS:HA	1:225:A:VAL:H	4	0.15
(1,2012)	1:277:A:LEU:HD11	1:478:A:SER:HA	15	0.14
(1,2012)	1:277:A:LEU:HD12	1:478:A:SER:HA	15	0.14
(1,2012)	1:277:A:LEU:HD13	1:478:A:SER:HA	15	0.14
(1,2012)	1:277:A:LEU:HD21	1:478:A:SER:HA	15	0.14
(1,2012)	1:277:A:LEU:HD22	1:478:A:SER:HA	15	0.14
(1,2012)	1:277:A:LEU:HD23	1:478:A:SER:HA	15	0.14
(1,1997)	1:475:A:VAL:H	1:476:A:PHE:HD1	9	0.14
(1,1984)	1:310:A:PHE:H	1:476:A:PHE:HE1	12	0.14
(1,1983)	1:228:A:MET:HE1	1:476:A:PHE:HE1	17	0.14
(1,1983)	1:228:A:MET:HE2	1:476:A:PHE:HE1	17	0.14
(1,1983)	1:228:A:MET:HE3	1:476:A:PHE:HE1	17	0.14
(1,1956)	1:226:A:TYR:HB2	1:475:A:VAL:HB	18	0.14
(1,1956)	1:226:A:TYR:HB3	1:475:A:VAL:HB	18	0.14
(1,1927)	1:400:A:LEU:HB2	1:474:A:LEU:HD21	6	0.14
(1,1927)	1:400:A:LEU:HB2	1:474:A:LEU:HD22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1927)	1:400:A:LEU:HB2	1:474:A:LEU:HD23	6	0.14
(1,1927)	1:400:A:LEU:HB3	1:474:A:LEU:HD21	6	0.14
(1,1927)	1:400:A:LEU:HB3	1:474:A:LEU:HD22	6	0.14
(1,1927)	1:400:A:LEU:HB3	1:474:A:LEU:HD23	6	0.14
(1,1851)	1:440:A:LEU:HD11	1:470:A:LEU:HG	15	0.14
(1,1851)	1:440:A:LEU:HD12	1:470:A:LEU:HG	15	0.14
(1,1851)	1:440:A:LEU:HD13	1:470:A:LEU:HG	15	0.14
(1,1851)	1:440:A:LEU:HD21	1:470:A:LEU:HG	15	0.14
(1,1851)	1:440:A:LEU:HD22	1:470:A:LEU:HG	15	0.14
(1,1851)	1:440:A:LEU:HD23	1:470:A:LEU:HG	15	0.14
(1,1835)	1:398:A:ASP:H	1:470:A:LEU:HG	15	0.14
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	3	0.14
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	3	0.14
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	3	0.14
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG21	8	0.14
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG22	8	0.14
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG23	8	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	6	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	6	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	6	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	18	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	18	0.14
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	18	0.14
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	15	0.14
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	15	0.14
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	15	0.14
(1,1804)	1:443:A:LEU:HD11	1:466:A:PRO:HA	19	0.14
(1,1804)	1:443:A:LEU:HD12	1:466:A:PRO:HA	19	0.14
(1,1804)	1:443:A:LEU:HD13	1:466:A:PRO:HA	19	0.14
(1,1804)	1:443:A:LEU:HD21	1:466:A:PRO:HA	19	0.14
(1,1804)	1:443:A:LEU:HD22	1:466:A:PRO:HA	19	0.14
(1,1804)	1:443:A:LEU:HD23	1:466:A:PRO:HA	19	0.14
(1,1783)	1:444:A:THR:HG21	1:445:A:GLU:H	19	0.14
(1,1783)	1:444:A:THR:HG22	1:445:A:GLU:H	19	0.14
(1,1783)	1:444:A:THR:HG23	1:445:A:GLU:H	19	0.14
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	3	0.14
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	12	0.14
(1,1631)	1:430:A:ARG:HB2	1:431:A:GLU:H	19	0.14
(1,1631)	1:430:A:ARG:HB3	1:431:A:GLU:H	19	0.14
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	2	0.14
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	2	0.14
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG2	3	0.14
(1,1618)	1:429:A:LEU:HG	1:430:A:ARG:HG3	3	0.14
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	4	0.14
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	4	0.14
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB2	12	0.14
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB3	12	0.14
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB2	12	0.14
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB3	12	0.14
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB2	12	0.14
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB3	12	0.14
(1,1548)	1:422:A:ILE:H	1:425:A:LEU:H	20	0.14
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE1	5	0.14
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE2	5	0.14
(1,1505)	1:392:A:TYR:HE1	1:403:A:MET:HE3	5	0.14
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB1	14	0.14
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB2	14	0.14
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB3	14	0.14
(1,1431)	1:394:A:PRO:HB2	1:396:A:GLU:H	17	0.14
(1,1431)	1:394:A:PRO:HB3	1:396:A:GLU:H	17	0.14
(1,1418)	1:333:A:ILE:HD11	1:392:A:TYR:HE1	6	0.14
(1,1418)	1:333:A:ILE:HD12	1:392:A:TYR:HE1	6	0.14
(1,1418)	1:333:A:ILE:HD13	1:392:A:TYR:HE1	6	0.14
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	11	0.14
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	11	0.14
(1,1410)	1:389:A:GLN:HE21	1:390:A:THR:HA	17	0.14
(1,1410)	1:389:A:GLN:HE22	1:390:A:THR:HA	17	0.14
(1,1409)	1:389:A:GLN:HG2	1:390:A:THR:HA	18	0.14
(1,1409)	1:389:A:GLN:HG3	1:390:A:THR:HA	18	0.14
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	8	0.14
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	8	0.14
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	8	0.14
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	8	0.14
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	17	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD11	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD12	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD13	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD21	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD22	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD23	3	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD11	3	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD12	3	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD13	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD21	3	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD22	3	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD23	3	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD11	10	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD12	10	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD13	10	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD21	10	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD22	10	0.14
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD23	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD11	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD12	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD13	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD21	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD22	10	0.14
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD23	10	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD11	5	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD12	5	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD13	5	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD21	5	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD22	5	0.14
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD23	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD11	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD12	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD13	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD21	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD22	5	0.14
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD23	5	0.14
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB2	10	0.14
(1,1352)	1:248:A:ARG:HD2	1:381:A:LEU:HB3	10	0.14
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB2	10	0.14
(1,1352)	1:248:A:ARG:HD3	1:381:A:LEU:HB3	10	0.14
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG2	7	0.14
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG3	7	0.14
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG2	17	0.14
(1,1321)	1:248:A:ARG:HH11	1:376:A:GLU:HG3	17	0.14
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG2	17	0.14
(1,1321)	1:248:A:ARG:HH12	1:376:A:GLU:HG3	17	0.14
(1,1298)	1:370:A:PRO:HB2	1:371:A:VAL:H	5	0.14
(1,1255)	1:357:A:ILE:HG21	1:359:A:ALA:HA	7	0.14
(1,1255)	1:357:A:ILE:HG22	1:359:A:ALA:HA	7	0.14
(1,1255)	1:357:A:ILE:HG23	1:359:A:ALA:HA	7	0.14
(1,1224)	1:354:A:VAL:HG21	1:355:A:PHE:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:354:A:VAL:HG22	1:355:A:PHE:H	19	0.14
(1,1224)	1:354:A:VAL:HG23	1:355:A:PHE:H	19	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG11	6	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG12	6	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG13	6	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG21	6	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG22	6	0.14
(1,1213)	1:352:A:PRO:HB2	1:354:A:VAL:HG23	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG11	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG12	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG13	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG21	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG22	6	0.14
(1,1213)	1:352:A:PRO:HB3	1:354:A:VAL:HG23	6	0.14
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	8	0.14
(1,1186)	1:348:A:LEU:H	1:349:A:ALA:HA	18	0.14
(1,1176)	1:341:A:THR:HA	1:349:A:ALA:HB1	15	0.14
(1,1176)	1:341:A:THR:HA	1:349:A:ALA:HB2	15	0.14
(1,1176)	1:341:A:THR:HA	1:349:A:ALA:HB3	15	0.14
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	4	0.14
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	11	0.14
(1,1154)	1:344:A:LYS:HG2	1:345:A:CYS:H	15	0.14
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB2	10	0.14
(1,1152)	1:342:A:GLY:HA2	1:345:A:CYS:HB3	10	0.14
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	17	0.14
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	20	0.14
(1,1103)	1:340:A:PHE:HB2	1:341:A:THR:H	2	0.14
(1,1103)	1:340:A:PHE:HB3	1:341:A:THR:H	2	0.14
(1,1103)	1:340:A:PHE:HB2	1:341:A:THR:H	6	0.14
(1,1103)	1:340:A:PHE:HB3	1:341:A:THR:H	6	0.14
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	10	0.14
(1,1063)	1:334:A:TYR:HA	1:337:A:THR:H	3	0.14
(1,1043)	1:335:A:GLU:H	1:336:A:LEU:HA	11	0.14
(1,990)	1:329:A:GLN:HB2	1:330:A:GLU:H	17	0.14
(1,990)	1:329:A:GLN:HB3	1:330:A:GLU:H	17	0.14
(1,980)	1:329:A:GLN:HB2	1:329:A:GLN:HE21	14	0.14
(1,980)	1:329:A:GLN:HB2	1:329:A:GLN:HE22	14	0.14
(1,980)	1:329:A:GLN:HB3	1:329:A:GLN:HE21	14	0.14
(1,980)	1:329:A:GLN:HB3	1:329:A:GLN:HE22	14	0.14
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	17	0.14
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	17	0.14
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	19	0.14
(1,923)	1:323:A:ILE:HA	1:324:A:TYR:H	7	0.14
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB2	15	0.14
(1,874)	1:319:A:ASP:HA	1:320:A:LYS:HB3	15	0.14
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	8	0.14
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	8	0.14
(1,792)	1:228:A:MET:HB2	1:309:A:CYS:HB2	17	0.14
(1,792)	1:228:A:MET:HB2	1:309:A:CYS:HB3	17	0.14
(1,792)	1:228:A:MET:HB3	1:309:A:CYS:HB2	17	0.14
(1,792)	1:228:A:MET:HB3	1:309:A:CYS:HB3	17	0.14
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	10	0.14
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	10	0.14
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	10	0.14
(1,772)	1:302:A:MET:HA	1:304:A:HIS:HD2	19	0.14
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	18	0.14
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	18	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD11	13	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD12	13	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD13	13	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD21	13	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD22	13	0.14
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD23	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD11	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD12	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD13	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD21	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD22	13	0.14
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD23	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD11	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD12	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD13	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD21	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD22	13	0.14
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD23	13	0.14
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	11	0.14
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	11	0.14
(1,706)	1:298:A:ILE:HD11	1:299:A:TYR:HE1	4	0.14
(1,706)	1:298:A:ILE:HD12	1:299:A:TYR:HE1	4	0.14
(1,706)	1:298:A:ILE:HD13	1:299:A:TYR:HE1	4	0.14
(1,665)	1:295:A:ILE:HG21	1:298:A:ILE:H	10	0.14
(1,665)	1:295:A:ILE:HG22	1:298:A:ILE:H	10	0.14
(1,665)	1:295:A:ILE:HG23	1:298:A:ILE:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	5	0.14
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	5	0.14
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	5	0.14
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD2	18	0.14
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD3	18	0.14
(1,653)	1:295:A:ILE:HG12	1:297:A:LYS:H	7	0.14
(1,653)	1:295:A:ILE:HG13	1:297:A:LYS:H	7	0.14
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	11	0.14
(1,633)	1:294:A:GLU:HG2	1:295:A:ILE:HG12	2	0.14
(1,633)	1:294:A:GLU:HG2	1:295:A:ILE:HG13	2	0.14
(1,633)	1:294:A:GLU:HG3	1:295:A:ILE:HG12	2	0.14
(1,633)	1:294:A:GLU:HG3	1:295:A:ILE:HG13	2	0.14
(1,627)	1:293:A:TYR:H	1:295:A:ILE:H	10	0.14
(1,627)	1:293:A:TYR:H	1:295:A:ILE:H	17	0.14
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD11	4	0.14
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD12	4	0.14
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD13	4	0.14
(1,563)	1:287:A:CYS:HA	1:292:A:ILE:H	6	0.14
(1,548)	1:287:A:CYS:HA	1:291:A:GLN:H	7	0.14
(1,520)	1:285:A:ASP:HB2	1:286:A:ASP:H	6	0.14
(1,491)	1:238:A:ILE:HD11	1:283:A:PRO:HA	16	0.14
(1,491)	1:238:A:ILE:HD12	1:283:A:PRO:HA	16	0.14
(1,491)	1:238:A:ILE:HD13	1:283:A:PRO:HA	16	0.14
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD11	2	0.14
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD12	2	0.14
(1,456)	1:274:A:PHE:H	1:281:A:ILE:HD13	2	0.14
(1,448)	1:238:A:ILE:HD11	1:281:A:ILE:HA	2	0.14
(1,448)	1:238:A:ILE:HD12	1:281:A:ILE:HA	2	0.14
(1,448)	1:238:A:ILE:HD13	1:281:A:ILE:HA	2	0.14
(1,435)	1:235:A:TYR:HB2	1:280:A:GLU:HB3	17	0.14
(1,435)	1:235:A:TYR:HB3	1:280:A:GLU:HB3	17	0.14
(1,422)	1:275:A:GLU:HA	1:279:A:PHE:H	9	0.14
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	10	0.14
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	18	0.14
(1,360)	1:273:A:THR:HG21	1:274:A:PHE:HE1	12	0.14
(1,360)	1:273:A:THR:HG22	1:274:A:PHE:HE1	12	0.14
(1,360)	1:273:A:THR:HG23	1:274:A:PHE:HE1	12	0.14
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	15	0.14
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	15	0.14
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	15	0.14
(1,343)	1:269:A:ALA:HA	1:273:A:THR:H	11	0.14
(1,301)	1:264:A:HIS:HB2	1:267:A:ALA:HB1	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:264:A:HIS:HB2	1:267:A:ALA:HB2	13	0.14
(1,301)	1:264:A:HIS:HB2	1:267:A:ALA:HB3	13	0.14
(1,301)	1:264:A:HIS:HB3	1:267:A:ALA:HB1	13	0.14
(1,301)	1:264:A:HIS:HB3	1:267:A:ALA:HB2	13	0.14
(1,301)	1:264:A:HIS:HB3	1:267:A:ALA:HB3	13	0.14
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	20	0.14
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB2	3	0.14
(1,282)	1:264:A:HIS:HD2	1:265:A:LEU:HB3	3	0.14
(1,267)	1:257:A:ILE:HA	1:258:A:ARG:H	3	0.14
(1,213)	1:251:A:VAL:H	1:254:A:LEU:HG	4	0.14
(1,191)	1:249:A:GLU:HB2	1:251:A:VAL:H	19	0.14
(1,191)	1:249:A:GLU:HB3	1:251:A:VAL:H	19	0.14
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG2	4	0.14
(1,177)	1:249:A:GLU:HB2	1:250:A:LYS:HG3	4	0.14
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG2	4	0.14
(1,177)	1:249:A:GLU:HB3	1:250:A:LYS:HG3	4	0.14
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB2	18	0.14
(1,166)	1:249:A:GLU:H	1:249:A:GLU:HB3	18	0.14
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD2	1	0.14
(1,135)	1:246:A:LYS:H	1:246:A:LYS:HD3	1	0.14
(1,127)	1:244:A:PHE:HA	1:245:A:ALA:H	14	0.14
(1,125)	1:243:A:ASN:HA	1:245:A:ALA:H	13	0.14
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	15	0.14
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	15	0.14
(1,43)	1:229:A:LYS:HA	1:229:A:LYS:HG2	8	0.14
(1,43)	1:229:A:LYS:HA	1:229:A:LYS:HG3	8	0.14
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	7	0.14
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	7	0.14
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	7	0.14
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	7	0.14
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE2	11	0.14
(1,40)	1:228:A:MET:HB2	1:229:A:LYS:HE3	11	0.14
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE2	11	0.14
(1,40)	1:228:A:MET:HB3	1:229:A:LYS:HE3	11	0.14
(1,1980)	1:474:A:LEU:HD11	1:475:A:VAL:H	5	0.13
(1,1980)	1:474:A:LEU:HD12	1:475:A:VAL:H	5	0.13
(1,1980)	1:474:A:LEU:HD13	1:475:A:VAL:H	5	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	20	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	20	0.13
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	20	0.13
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE2	20	0.13
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE3	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	4	0.13
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	4	0.13
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	4	0.13
(1,1827)	1:468:A:PHE:HB2	1:469:A:THR:H	13	0.13
(1,1795)	1:444:A:THR:HG21	1:446:A:VAL:H	18	0.13
(1,1795)	1:444:A:THR:HG22	1:446:A:VAL:H	18	0.13
(1,1795)	1:444:A:THR:HG23	1:446:A:VAL:H	18	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD11	14	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD12	14	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD13	14	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD21	14	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD22	14	0.13
(1,1763)	1:442:A:ILE:HB	1:443:A:LEU:HD23	14	0.13
(1,1759)	1:439:A:ILE:HA	1:443:A:LEU:H	1	0.13
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD11	1	0.13
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD12	1	0.13
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD13	1	0.13
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG2	10	0.13
(1,1658)	1:434:A:PRO:HA	1:435:A:ARG:HG3	10	0.13
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD2	4	0.13
(1,1650)	1:432:A:ARG:H	1:434:A:PRO:HD3	4	0.13
(1,1640)	1:273:A:THR:HG21	1:433:A:CYS:H	18	0.13
(1,1640)	1:273:A:THR:HG22	1:433:A:CYS:H	18	0.13
(1,1640)	1:273:A:THR:HG23	1:433:A:CYS:H	18	0.13
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB2	13	0.13
(1,1636)	1:430:A:ARG:HD2	1:431:A:GLU:HB3	13	0.13
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB2	13	0.13
(1,1636)	1:430:A:ARG:HD3	1:431:A:GLU:HB3	13	0.13
(1,1630)	1:429:A:LEU:HD11	1:431:A:GLU:H	5	0.13
(1,1630)	1:429:A:LEU:HD12	1:431:A:GLU:H	5	0.13
(1,1630)	1:429:A:LEU:HD13	1:431:A:GLU:H	5	0.13
(1,1609)	1:273:A:THR:HG21	1:430:A:ARG:HG2	14	0.13
(1,1609)	1:273:A:THR:HG21	1:430:A:ARG:HG3	14	0.13
(1,1609)	1:273:A:THR:HG22	1:430:A:ARG:HG2	14	0.13
(1,1609)	1:273:A:THR:HG22	1:430:A:ARG:HG3	14	0.13
(1,1609)	1:273:A:THR:HG23	1:430:A:ARG:HG2	14	0.13
(1,1609)	1:273:A:THR:HG23	1:430:A:ARG:HG3	14	0.13
(1,1595)	1:428:A:SER:H	1:429:A:LEU:HG	11	0.13
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD11	17	0.13
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD12	17	0.13
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD13	17	0.13
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD21	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD22	17	0.13
(1,1551)	1:422:A:ILE:H	1:425:A:LEU:HD23	17	0.13
(1,1548)	1:422:A:ILE:H	1:425:A:LEU:H	1	0.13
(1,1509)	1:401:A:LEU:HG	1:403:A:MET:HE1	4	0.13
(1,1509)	1:401:A:LEU:HG	1:403:A:MET:HE2	4	0.13
(1,1509)	1:401:A:LEU:HG	1:403:A:MET:HE3	4	0.13
(1,1502)	1:357:A:ILE:HD11	1:403:A:MET:HG2	20	0.13
(1,1502)	1:357:A:ILE:HD11	1:403:A:MET:HG3	20	0.13
(1,1502)	1:357:A:ILE:HD12	1:403:A:MET:HG2	20	0.13
(1,1502)	1:357:A:ILE:HD12	1:403:A:MET:HG3	20	0.13
(1,1502)	1:357:A:ILE:HD13	1:403:A:MET:HG2	20	0.13
(1,1502)	1:357:A:ILE:HD13	1:403:A:MET:HG3	20	0.13
(1,1482)	1:400:A:LEU:HG	1:401:A:LEU:H	19	0.13
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	10	0.13
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	10	0.13
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	10	0.13
(1,1453)	1:397:A:ALA:HB1	1:399:A:PHE:H	19	0.13
(1,1453)	1:397:A:ALA:HB2	1:399:A:PHE:H	19	0.13
(1,1453)	1:397:A:ALA:HB3	1:399:A:PHE:H	19	0.13
(1,1450)	1:397:A:ALA:HB1	1:398:A:ASP:HB2	10	0.13
(1,1450)	1:397:A:ALA:HB1	1:398:A:ASP:HB3	10	0.13
(1,1450)	1:397:A:ALA:HB2	1:398:A:ASP:HB2	10	0.13
(1,1450)	1:397:A:ALA:HB2	1:398:A:ASP:HB3	10	0.13
(1,1450)	1:397:A:ALA:HB3	1:398:A:ASP:HB2	10	0.13
(1,1450)	1:397:A:ALA:HB3	1:398:A:ASP:HB3	10	0.13
(1,1448)	1:397:A:ALA:HB1	1:398:A:ASP:H	8	0.13
(1,1448)	1:397:A:ALA:HB2	1:398:A:ASP:H	8	0.13
(1,1448)	1:397:A:ALA:HB3	1:398:A:ASP:H	8	0.13
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB1	9	0.13
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB2	9	0.13
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB3	9	0.13
(1,1436)	1:395:A:ASP:HA	1:396:A:GLU:H	3	0.13
(1,1415)	1:320:A:LYS:HD2	1:392:A:TYR:HD1	5	0.13
(1,1415)	1:320:A:LYS:HD3	1:392:A:TYR:HD1	5	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	2	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	2	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	4	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	4	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	19	0.13
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	19	0.13
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	3	0.13
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	3	0.13
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	3	0.13
(1,1377)	1:381:A:LEU:H	1:381:A:LEU:HB2	18	0.13
(1,1377)	1:381:A:LEU:H	1:381:A:LEU:HB3	18	0.13
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB2	5	0.13
(1,1343)	1:376:A:GLU:HB2	1:380:A:TYR:HB3	5	0.13
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB2	5	0.13
(1,1343)	1:376:A:GLU:HB3	1:380:A:TYR:HB3	5	0.13
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG21	8	0.13
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG22	8	0.13
(1,1313)	1:248:A:ARG:HD2	1:373:A:THR:HG23	8	0.13
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG21	8	0.13
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG22	8	0.13
(1,1313)	1:248:A:ARG:HD3	1:373:A:THR:HG23	8	0.13
(1,1312)	1:248:A:ARG:HG2	1:373:A:THR:HB	16	0.13
(1,1312)	1:248:A:ARG:HG3	1:373:A:THR:HB	16	0.13
(1,1311)	1:248:A:ARG:HG2	1:373:A:THR:HG21	15	0.13
(1,1311)	1:248:A:ARG:HG2	1:373:A:THR:HG22	15	0.13
(1,1311)	1:248:A:ARG:HG2	1:373:A:THR:HG23	15	0.13
(1,1311)	1:248:A:ARG:HG3	1:373:A:THR:HG21	15	0.13
(1,1311)	1:248:A:ARG:HG3	1:373:A:THR:HG22	15	0.13
(1,1311)	1:248:A:ARG:HG3	1:373:A:THR:HG23	15	0.13
(1,1298)	1:370:A:PRO:HB2	1:371:A:VAL:H	20	0.13
(1,1259)	1:359:A:ALA:H	1:360:A:ALA:HB1	10	0.13
(1,1259)	1:359:A:ALA:H	1:360:A:ALA:HB2	10	0.13
(1,1259)	1:359:A:ALA:H	1:360:A:ALA:HB3	10	0.13
(1,1250)	1:357:A:ILE:HA	1:358:A:GLN:H	19	0.13
(1,1234)	1:313:A:CYS:HA	1:356:A:PHE:H	15	0.13
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	4	0.13
(1,1167)	1:346:A:PRO:HA	1:348:A:LEU:H	4	0.13
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	17	0.13
(1,1161)	1:345:A:CYS:H	1:346:A:PRO:HA	15	0.13
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	1	0.13
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	6	0.13
(1,1126)	1:341:A:THR:H	1:344:A:LYS:H	3	0.13
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	4	0.13
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	4	0.13
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	12	0.13
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	12	0.13
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	12	0.13
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	12	0.13
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	12	0.13
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	4	0.13
(1,1091)	1:338:A:SER:HA	1:340:A:PHE:H	20	0.13
(1,1072)	1:336:A:LEU:HG	1:337:A:THR:H	9	0.13
(1,1072)	1:336:A:LEU:HG	1:337:A:THR:H	20	0.13
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB2	11	0.13
(1,1046)	1:335:A:GLU:H	1:336:A:LEU:HB3	11	0.13
(1,1019)	1:333:A:ILE:H	1:335:A:GLU:H	9	0.13
(1,1016)	1:334:A:TYR:HB2	1:334:A:TYR:HE1	16	0.13
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	20	0.13
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB1	7	0.13
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB2	7	0.13
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB3	7	0.13
(1,987)	1:324:A:TYR:HA	1:330:A:GLU:HA	4	0.13
(1,987)	1:324:A:TYR:HA	1:330:A:GLU:HA	20	0.13
(1,967)	1:289:A:VAL:HG11	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG11	1:329:A:GLN:HG3	18	0.13
(1,967)	1:289:A:VAL:HG12	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG12	1:329:A:GLN:HG3	18	0.13
(1,967)	1:289:A:VAL:HG13	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG13	1:329:A:GLN:HG3	18	0.13
(1,967)	1:289:A:VAL:HG21	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG21	1:329:A:GLN:HG3	18	0.13
(1,967)	1:289:A:VAL:HG22	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG22	1:329:A:GLN:HG3	18	0.13
(1,967)	1:289:A:VAL:HG23	1:329:A:GLN:HG2	18	0.13
(1,967)	1:289:A:VAL:HG23	1:329:A:GLN:HG3	18	0.13
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	14	0.13
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	14	0.13
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG21	9	0.13
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG22	9	0.13
(1,934)	1:246:A:LYS:H	1:326:A:THR:HG23	9	0.13
(1,926)	1:323:A:ILE:HG21	1:324:A:TYR:HD1	20	0.13
(1,926)	1:323:A:ILE:HG22	1:324:A:TYR:HD1	20	0.13
(1,926)	1:323:A:ILE:HG23	1:324:A:TYR:HD1	20	0.13
(1,885)	1:319:A:ASP:H	1:322:A:ILE:H	17	0.13
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	15	0.13
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	15	0.13
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE2	17	0.13
(1,882)	1:320:A:LYS:HA	1:320:A:LYS:HE3	17	0.13
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	9	0.13
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	9	0.13
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	9	0.13
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	20	0.13
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	20	0.13
(1,844)	1:313:A:CYS:H	1:314:A:ILE:H	18	0.13
(1,839)	1:312:A:CYS:H	1:313:A:CYS:H	20	0.13
(1,785)	1:306:A:ASN:H	1:307:A:MET:H	16	0.13
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	7	0.13
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	7	0.13
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	7	0.13
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	1	0.13
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	13	0.13
(1,775)	1:303:A:ASP:H	1:304:A:HIS:HD2	13	0.13
(1,741)	1:299:A:TYR:HD1	1:302:A:MET:HE1	7	0.13
(1,741)	1:299:A:TYR:HD1	1:302:A:MET:HE2	7	0.13
(1,741)	1:299:A:TYR:HD1	1:302:A:MET:HE3	7	0.13
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	15	0.13
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	15	0.13
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	15	0.13
(1,723)	1:298:A:ILE:HG21	1:301:A:LEU:HG	20	0.13
(1,723)	1:298:A:ILE:HG22	1:301:A:LEU:HG	20	0.13
(1,723)	1:298:A:ILE:HG23	1:301:A:LEU:HG	20	0.13
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	2	0.13
(1,709)	1:299:A:TYR:H	1:299:A:TYR:HE1	20	0.13
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	6	0.13
(1,707)	1:298:A:ILE:HB	1:299:A:TYR:HE1	14	0.13
(1,697)	1:297:A:LYS:HA	1:299:A:TYR:H	5	0.13
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	12	0.13
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	12	0.13
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	12	0.13
(1,653)	1:295:A:ILE:HG12	1:297:A:LYS:H	6	0.13
(1,653)	1:295:A:ILE:HG13	1:297:A:LYS:H	6	0.13
(1,653)	1:295:A:ILE:HG12	1:297:A:LYS:H	12	0.13
(1,653)	1:295:A:ILE:HG13	1:297:A:LYS:H	12	0.13
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	5	0.13
(1,627)	1:293:A:TYR:H	1:295:A:ILE:H	9	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD11	11	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD12	11	0.13
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD13	11	0.13
(1,567)	1:287:A:CYS:HB2	1:292:A:ILE:H	13	0.13
(1,567)	1:287:A:CYS:HB3	1:292:A:ILE:H	13	0.13
(1,548)	1:287:A:CYS:HA	1:291:A:GLN:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:238:A:ILE:H	1:284:A:HIS:HD2	2	0.13
(1,494)	1:238:A:ILE:H	1:284:A:HIS:HD2	11	0.13
(1,438)	1:235:A:TYR:HA	1:280:A:GLU:HB2	8	0.13
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	7	0.13
(1,397)	1:275:A:GLU:H	1:277:A:LEU:H	14	0.13
(1,371)	1:272:A:THR:HA	1:275:A:GLU:HA	10	0.13
(1,274)	1:258:A:ARG:HA	1:258:A:ARG:HD2	4	0.13
(1,274)	1:258:A:ARG:HA	1:258:A:ARG:HD3	4	0.13
(1,187)	1:247:A:ALA:HB1	1:251:A:VAL:H	7	0.13
(1,187)	1:247:A:ALA:HB2	1:251:A:VAL:H	7	0.13
(1,187)	1:247:A:ALA:HB3	1:251:A:VAL:H	7	0.13
(1,146)	1:245:A:ALA:H	1:247:A:ALA:H	18	0.13
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE2	17	0.13
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE3	17	0.13
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	17	0.13
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE2	19	0.13
(1,58)	1:231:A:LYS:HA	1:231:A:LYS:HE3	19	0.13
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG2	8	0.13
(1,36)	1:227:A:GLN:HG2	1:229:A:LYS:HG3	8	0.13
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG2	8	0.13
(1,36)	1:227:A:GLN:HG3	1:229:A:LYS:HG3	8	0.13
(1,2017)	1:277:A:LEU:HD11	1:479:A:ASP:H	17	0.12
(1,2017)	1:277:A:LEU:HD12	1:479:A:ASP:H	17	0.12
(1,2017)	1:277:A:LEU:HD13	1:479:A:ASP:H	17	0.12
(1,2017)	1:277:A:LEU:HD21	1:479:A:ASP:H	17	0.12
(1,2017)	1:277:A:LEU:HD22	1:479:A:ASP:H	17	0.12
(1,2017)	1:277:A:LEU:HD23	1:479:A:ASP:H	17	0.12
(1,1972)	1:473:A:LYS:HE2	1:475:A:VAL:H	7	0.12
(1,1972)	1:473:A:LYS:HE3	1:475:A:VAL:H	7	0.12
(1,1972)	1:473:A:LYS:HE2	1:475:A:VAL:H	14	0.12
(1,1972)	1:473:A:LYS:HE3	1:475:A:VAL:H	14	0.12
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	7	0.12
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	7	0.12
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	7	0.12
(1,1892)	1:225:A:VAL:HB	1:473:A:LYS:HA	11	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD11	6	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD12	6	0.12
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD13	6	0.12
(1,1834)	1:398:A:ASP:H	1:470:A:LEU:HA	20	0.12
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	15	0.12
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	15	0.12
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG21	17	0.12
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG22	17	0.12
(1,1830)	1:468:A:PHE:HB2	1:469:A:THR:HG23	17	0.12
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	5	0.12
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	5	0.12
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	5	0.12
(1,1814)	1:401:A:LEU:H	1:468:A:PHE:HB3	15	0.12
(1,1795)	1:444:A:THR:HG21	1:446:A:VAL:H	20	0.12
(1,1795)	1:444:A:THR:HG22	1:446:A:VAL:H	20	0.12
(1,1795)	1:444:A:THR:HG23	1:446:A:VAL:H	20	0.12
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG21	1	0.12
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG22	1	0.12
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG23	1	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD22	12	0.12
(1,1758)	1:425:A:LEU:HD11	1:443:A:LEU:HD23	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD22	12	0.12
(1,1758)	1:425:A:LEU:HD12	1:443:A:LEU:HD23	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD22	12	0.12
(1,1758)	1:425:A:LEU:HD13	1:443:A:LEU:HD23	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD22	12	0.12
(1,1758)	1:425:A:LEU:HD21	1:443:A:LEU:HD23	12	0.12
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD22	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:425:A:LEU:HD22	1:443:A:LEU:HD23	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD11	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD12	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD13	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD21	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD22	12	0.12
(1,1758)	1:425:A:LEU:HD23	1:443:A:LEU:HD23	12	0.12
(1,1742)	1:442:A:ILE:H	1:442:A:ILE:HD11	10	0.12
(1,1742)	1:442:A:ILE:H	1:442:A:ILE:HD12	10	0.12
(1,1742)	1:442:A:ILE:H	1:442:A:ILE:HD13	10	0.12
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD11	8	0.12
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD12	8	0.12
(1,1737)	1:439:A:ILE:HA	1:442:A:ILE:HD13	8	0.12
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG21	3	0.12
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG22	3	0.12
(1,1725)	1:428:A:SER:HB2	1:442:A:ILE:HG23	3	0.12
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG21	3	0.12
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG22	3	0.12
(1,1725)	1:428:A:SER:HB3	1:442:A:ILE:HG23	3	0.12
(1,1718)	1:439:A:ILE:H	1:441:A:THR:H	11	0.12
(1,1705)	1:439:A:ILE:HG21	1:440:A:LEU:H	19	0.12
(1,1705)	1:439:A:ILE:HG22	1:440:A:LEU:H	19	0.12
(1,1705)	1:439:A:ILE:HG23	1:440:A:LEU:H	19	0.12
(1,1679)	1:436:A:GLY:H	1:437:A:ASP:HB2	10	0.12
(1,1679)	1:436:A:GLY:H	1:437:A:ASP:HB3	10	0.12
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	14	0.12
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	14	0.12
(1,1564)	1:424:A:SER:HB2	1:426:A:CYS:H	9	0.12
(1,1564)	1:424:A:SER:HB3	1:426:A:CYS:H	9	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD11	8	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD12	8	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD13	8	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD21	8	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD22	8	0.12
(1,1546)	1:356:A:PHE:HE1	1:425:A:LEU:HD23	8	0.12
(1,1516)	1:403:A:MET:HG2	1:404:A:ALA:H	18	0.12
(1,1516)	1:403:A:MET:HG3	1:404:A:ALA:H	18	0.12
(1,1499)	1:357:A:ILE:HA	1:403:A:MET:HE1	19	0.12
(1,1499)	1:357:A:ILE:HA	1:403:A:MET:HE2	19	0.12
(1,1499)	1:357:A:ILE:HA	1:403:A:MET:HE3	19	0.12
(1,1496)	1:401:A:LEU:HA	1:402:A:GLY:H	11	0.12
(1,1489)	1:356:A:PHE:HA	1:402:A:GLY:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:396:A:GLU:H	1:396:A:GLU:HG2	10	0.12
(1,1439)	1:396:A:GLU:H	1:396:A:GLU:HG3	10	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD11	16	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD12	16	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD13	16	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD21	16	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD22	16	0.12
(1,1400)	1:384:A:ASP:HB2	1:385:A:LEU:HD23	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD11	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD12	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD13	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD21	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD22	16	0.12
(1,1400)	1:384:A:ASP:HB3	1:385:A:LEU:HD23	16	0.12
(1,1394)	1:384:A:ASP:H	1:385:A:LEU:HA	3	0.12
(1,1394)	1:384:A:ASP:H	1:385:A:LEU:HA	4	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	6	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	6	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	11	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	11	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	16	0.12
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	16	0.12
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG2	12	0.12
(1,1385)	1:381:A:LEU:HB2	1:382:A:GLU:HG3	12	0.12
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG2	12	0.12
(1,1385)	1:381:A:LEU:HB3	1:382:A:GLU:HG3	12	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD11	4	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD12	4	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD13	4	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD21	4	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD22	4	0.12
(1,1363)	1:376:A:GLU:HG2	1:381:A:LEU:HD23	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD11	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD12	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD13	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD21	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD22	4	0.12
(1,1363)	1:376:A:GLU:HG3	1:381:A:LEU:HD23	4	0.12
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD11	9	0.12
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD12	9	0.12
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD13	9	0.12
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD22	9	0.12
(1,1360)	1:376:A:GLU:HA	1:381:A:LEU:HD23	9	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD11	1	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD12	1	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD13	1	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD21	1	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD22	1	0.12
(1,1354)	1:249:A:GLU:HG2	1:381:A:LEU:HD23	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD11	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD12	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD13	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD21	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD22	1	0.12
(1,1354)	1:249:A:GLU:HG3	1:381:A:LEU:HD23	1	0.12
(1,1328)	1:377:A:GLU:HA	1:378:A:GLN:HA	12	0.12
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG2	4	0.12
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG3	4	0.12
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG2	14	0.12
(1,1323)	1:376:A:GLU:HA	1:376:A:GLU:HG3	14	0.12
(1,1320)	1:248:A:ARG:HD2	1:376:A:GLU:HA	13	0.12
(1,1320)	1:248:A:ARG:HD3	1:376:A:GLU:HA	13	0.12
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	12	0.12
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	12	0.12
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	6	0.12
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	6	0.12
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	8	0.12
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	8	0.12
(1,1280)	1:369:A:ILE:H	1:369:A:ILE:HB	4	0.12
(1,1280)	1:369:A:ILE:H	1:369:A:ILE:HB	15	0.12
(1,1235)	1:313:A:CYS:HB2	1:356:A:PHE:H	6	0.12
(1,1235)	1:313:A:CYS:HB3	1:356:A:PHE:H	6	0.12
(1,1199)	1:310:A:PHE:H	1:354:A:VAL:H	14	0.12
(1,1191)	1:348:A:LEU:HD11	1:351:A:LYS:H	3	0.12
(1,1191)	1:348:A:LEU:HD12	1:351:A:LYS:H	3	0.12
(1,1191)	1:348:A:LEU:HD13	1:351:A:LYS:H	3	0.12
(1,1191)	1:348:A:LEU:HD21	1:351:A:LYS:H	3	0.12
(1,1191)	1:348:A:LEU:HD22	1:351:A:LYS:H	3	0.12
(1,1191)	1:348:A:LEU:HD23	1:351:A:LYS:H	3	0.12
(1,1154)	1:344:A:LYS:HG2	1:345:A:CYS:H	4	0.12
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	2	0.12
(1,1147)	1:341:A:THR:HG21	1:345:A:CYS:H	12	0.12
(1,1147)	1:341:A:THR:HG22	1:345:A:CYS:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:341:A:THR:HG23	1:345:A:CYS:H	12	0.12
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE2	13	0.12
(1,1136)	1:343:A:LEU:HB3	1:344:A:LYS:HE3	13	0.12
(1,1103)	1:340:A:PHE:HB2	1:341:A:THR:H	19	0.12
(1,1103)	1:340:A:PHE:HB3	1:341:A:THR:H	19	0.12
(1,1079)	1:337:A:THR:HG21	1:338:A:SER:H	11	0.12
(1,1079)	1:337:A:THR:HG22	1:338:A:SER:H	11	0.12
(1,1079)	1:337:A:THR:HG23	1:338:A:SER:H	11	0.12
(1,1067)	1:336:A:LEU:H	1:337:A:THR:HG21	4	0.12
(1,1067)	1:336:A:LEU:H	1:337:A:THR:HG22	4	0.12
(1,1067)	1:336:A:LEU:H	1:337:A:THR:HG23	4	0.12
(1,1061)	1:333:A:ILE:HB	1:337:A:THR:HG21	9	0.12
(1,1061)	1:333:A:ILE:HB	1:337:A:THR:HG22	9	0.12
(1,1061)	1:333:A:ILE:HB	1:337:A:THR:HG23	9	0.12
(1,1058)	1:296:A:LEU:HD11	1:337:A:THR:HB	15	0.12
(1,1058)	1:296:A:LEU:HD12	1:337:A:THR:HB	15	0.12
(1,1058)	1:296:A:LEU:HD13	1:337:A:THR:HB	15	0.12
(1,1058)	1:296:A:LEU:HD21	1:337:A:THR:HB	15	0.12
(1,1058)	1:296:A:LEU:HD22	1:337:A:THR:HB	15	0.12
(1,1058)	1:296:A:LEU:HD23	1:337:A:THR:HB	15	0.12
(1,1043)	1:335:A:GLU:H	1:336:A:LEU:HA	13	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	3	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	3	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	3	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD11	18	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD12	18	0.12
(1,1042)	1:334:A:TYR:H	1:336:A:LEU:HD13	18	0.12
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	18	0.12
(1,1038)	1:333:A:ILE:HG21	1:336:A:LEU:H	9	0.12
(1,1038)	1:333:A:ILE:HG22	1:336:A:LEU:H	9	0.12
(1,1038)	1:333:A:ILE:HG23	1:336:A:LEU:H	9	0.12
(1,1018)	1:333:A:ILE:HG21	1:335:A:GLU:H	11	0.12
(1,1018)	1:333:A:ILE:HG22	1:335:A:GLU:H	11	0.12
(1,1018)	1:333:A:ILE:HG23	1:335:A:GLU:H	11	0.12
(1,1016)	1:334:A:TYR:HB2	1:334:A:TYR:HE1	18	0.12
(1,986)	1:289:A:VAL:HG11	1:330:A:GLU:HA	10	0.12
(1,986)	1:289:A:VAL:HG12	1:330:A:GLU:HA	10	0.12
(1,986)	1:289:A:VAL:HG13	1:330:A:GLU:HA	10	0.12
(1,986)	1:289:A:VAL:HG21	1:330:A:GLU:HA	10	0.12
(1,986)	1:289:A:VAL:HG22	1:330:A:GLU:HA	10	0.12
(1,986)	1:289:A:VAL:HG23	1:330:A:GLU:HA	10	0.12
(1,958)	1:326:A:THR:HG21	1:328:A:GLY:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:326:A:THR:HG22	1:328:A:GLY:H	12	0.12
(1,958)	1:326:A:THR:HG23	1:328:A:GLY:H	12	0.12
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA2	3	0.12
(1,957)	1:318:A:GLY:H	1:328:A:GLY:HA3	3	0.12
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA2	20	0.12
(1,954)	1:250:A:LYS:HD2	1:328:A:GLY:HA3	20	0.12
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA2	20	0.12
(1,954)	1:250:A:LYS:HD3	1:328:A:GLY:HA3	20	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG21	14	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG22	14	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG23	14	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG21	16	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG22	16	0.12
(1,938)	1:326:A:THR:H	1:326:A:THR:HG23	16	0.12
(1,930)	1:324:A:TYR:HD1	1:325:A:GLY:H	6	0.12
(1,926)	1:323:A:ILE:HG21	1:324:A:TYR:HD1	13	0.12
(1,926)	1:323:A:ILE:HG22	1:324:A:TYR:HD1	13	0.12
(1,926)	1:323:A:ILE:HG23	1:324:A:TYR:HD1	13	0.12
(1,891)	1:319:A:ASP:HA	1:322:A:ILE:HD11	19	0.12
(1,891)	1:319:A:ASP:HA	1:322:A:ILE:HD12	19	0.12
(1,891)	1:319:A:ASP:HA	1:322:A:ILE:HD13	19	0.12
(1,886)	1:319:A:ASP:H	1:322:A:ILE:HB	2	0.12
(1,886)	1:319:A:ASP:H	1:322:A:ILE:HB	8	0.12
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD2	9	0.12
(1,883)	1:320:A:LYS:HA	1:320:A:LYS:HD3	9	0.12
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	14	0.12
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	14	0.12
(1,865)	1:239:A:ILE:HG21	1:316:A:SER:H	18	0.12
(1,865)	1:239:A:ILE:HG22	1:316:A:SER:H	18	0.12
(1,865)	1:239:A:ILE:HG23	1:316:A:SER:H	18	0.12
(1,842)	1:313:A:CYS:H	1:314:A:ILE:HD11	18	0.12
(1,842)	1:313:A:CYS:H	1:314:A:ILE:HD12	18	0.12
(1,842)	1:313:A:CYS:H	1:314:A:ILE:HD13	18	0.12
(1,805)	1:236:A:CYS:HA	1:311:A:ILE:H	11	0.12
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	17	0.12
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE1	16	0.12
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE2	16	0.12
(1,788)	1:307:A:MET:HB2	1:307:A:MET:HE3	16	0.12
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE1	16	0.12
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE2	16	0.12
(1,788)	1:307:A:MET:HB3	1:307:A:MET:HE3	16	0.12
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	14	0.12
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	14	0.12
(1,781)	1:305:A:SER:H	1:306:A:ASN:HA	18	0.12
(1,762)	1:300:A:GLN:H	1:303:A:ASP:H	11	0.12
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	7	0.12
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	7	0.12
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	18	0.12
(1,712)	1:297:A:LYS:H	1:300:A:GLN:H	18	0.12
(1,695)	1:295:A:ILE:HG21	1:299:A:TYR:HD1	15	0.12
(1,695)	1:295:A:ILE:HG22	1:299:A:TYR:HD1	15	0.12
(1,695)	1:295:A:ILE:HG23	1:299:A:TYR:HD1	15	0.12
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD11	14	0.12
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD12	14	0.12
(1,672)	1:295:A:ILE:HG21	1:298:A:ILE:HD13	14	0.12
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD11	14	0.12
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD12	14	0.12
(1,672)	1:295:A:ILE:HG22	1:298:A:ILE:HD13	14	0.12
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD11	14	0.12
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD12	14	0.12
(1,672)	1:295:A:ILE:HG23	1:298:A:ILE:HD13	14	0.12
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD2	10	0.12
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD3	10	0.12
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	1	0.12
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	3	0.12
(1,641)	1:293:A:TYR:HD1	1:296:A:LEU:H	4	0.12
(1,605)	1:292:A:ILE:HB	1:293:A:TYR:HD1	2	0.12
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	18	0.12
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	1	0.12
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	1	0.12
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	1	0.12
(1,516)	1:241:A:ASN:HB2	1:286:A:ASP:HA	6	0.12
(1,516)	1:241:A:ASN:HB3	1:286:A:ASP:HA	6	0.12
(1,501)	1:240:A:ASN:HB2	1:284:A:HIS:H	6	0.12
(1,501)	1:240:A:ASN:HB3	1:284:A:HIS:H	6	0.12
(1,501)	1:240:A:ASN:HB2	1:284:A:HIS:H	19	0.12
(1,501)	1:240:A:ASN:HB3	1:284:A:HIS:H	19	0.12
(1,433)	1:235:A:TYR:HA	1:280:A:GLU:H	17	0.12
(1,431)	1:279:A:PHE:H	1:279:A:PHE:HD1	15	0.12
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	11	0.12
(1,420)	1:234:A:GLY:H	1:279:A:PHE:HA	13	0.12
(1,413)	1:276:A:GLU:H	1:278:A:HIS:H	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD11	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD12	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD13	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD21	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD22	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD23	10	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD11	19	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD12	19	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD13	19	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD21	19	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD22	19	0.12
(1,399)	1:275:A:GLU:H	1:277:A:LEU:HD23	19	0.12
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG2	10	0.12
(1,374)	1:272:A:THR:H	1:275:A:GLU:HG3	10	0.12
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	5	0.12
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	5	0.12
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	5	0.12
(1,339)	1:271:A:THR:HG21	1:272:A:THR:HA	10	0.12
(1,339)	1:271:A:THR:HG22	1:272:A:THR:HA	10	0.12
(1,339)	1:271:A:THR:HG23	1:272:A:THR:HA	10	0.12
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	15	0.12
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	20	0.12
(1,268)	1:257:A:ILE:HB	1:258:A:ARG:H	3	0.12
(1,267)	1:257:A:ILE:HA	1:258:A:ARG:H	6	0.12
(1,252)	1:254:A:LEU:HB2	1:257:A:ILE:HD11	1	0.12
(1,252)	1:254:A:LEU:HB2	1:257:A:ILE:HD12	1	0.12
(1,252)	1:254:A:LEU:HB2	1:257:A:ILE:HD13	1	0.12
(1,252)	1:254:A:LEU:HB3	1:257:A:ILE:HD11	1	0.12
(1,252)	1:254:A:LEU:HB3	1:257:A:ILE:HD12	1	0.12
(1,252)	1:254:A:LEU:HB3	1:257:A:ILE:HD13	1	0.12
(1,235)	1:253:A:LYS:HA	1:255:A:HIS:HD2	6	0.12
(1,215)	1:251:A:VAL:H	1:254:A:LEU:H	18	0.12
(1,211)	1:247:A:ALA:HB1	1:254:A:LEU:HG	7	0.12
(1,211)	1:247:A:ALA:HB2	1:254:A:LEU:HG	7	0.12
(1,211)	1:247:A:ALA:HB3	1:254:A:LEU:HG	7	0.12
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD2	4	0.12
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD3	4	0.12
(1,180)	1:250:A:LYS:HA	1:250:A:LYS:HD2	19	0.12
(1,180)	1:250:A:LYS:HA	1:250:A:LYS:HD3	19	0.12
(1,175)	1:249:A:GLU:HB2	1:250:A:LYS:H	7	0.12
(1,175)	1:249:A:GLU:HB3	1:250:A:LYS:H	7	0.12
(1,161)	1:247:A:ALA:HB1	1:249:A:GLU:H	3	0.12
(1,161)	1:247:A:ALA:HB2	1:249:A:GLU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:247:A:ALA:HB3	1:249:A:GLU:H	3	0.12
(1,151)	1:246:A:LYS:H	1:248:A:ARG:H	19	0.12
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE2	3	0.12
(1,133)	1:246:A:LYS:H	1:246:A:LYS:HE3	3	0.12
(1,120)	1:242:A:HIS:HB2	1:243:A:ASN:H	19	0.12
(1,120)	1:242:A:HIS:HB3	1:243:A:ASN:H	19	0.12
(1,118)	1:241:A:ASN:HA	1:243:A:ASN:H	3	0.12
(1,74)	1:235:A:TYR:H	1:235:A:TYR:HD1	14	0.12
(1,65)	1:231:A:LYS:HG2	1:232:A:PRO:HA	2	0.12
(1,65)	1:231:A:LYS:HG3	1:232:A:PRO:HA	2	0.12
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD2	9	0.12
(1,54)	1:231:A:LYS:H	1:231:A:LYS:HD3	9	0.12
(1,48)	1:229:A:LYS:HG2	1:230:A:SER:H	9	0.12
(1,48)	1:229:A:LYS:HG3	1:230:A:SER:H	9	0.12
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE2	7	0.12
(1,44)	1:229:A:LYS:HA	1:229:A:LYS:HE3	7	0.12
(1,2013)	1:277:A:LEU:HD11	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD11	1:478:A:SER:HB3	16	0.11
(1,2013)	1:277:A:LEU:HD12	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD12	1:478:A:SER:HB3	16	0.11
(1,2013)	1:277:A:LEU:HD13	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD13	1:478:A:SER:HB3	16	0.11
(1,2013)	1:277:A:LEU:HD21	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD21	1:478:A:SER:HB3	16	0.11
(1,2013)	1:277:A:LEU:HD22	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD22	1:478:A:SER:HB3	16	0.11
(1,2013)	1:277:A:LEU:HD23	1:478:A:SER:HB2	16	0.11
(1,2013)	1:277:A:LEU:HD23	1:478:A:SER:HB3	16	0.11
(1,1984)	1:310:A:PHE:H	1:476:A:PHE:HE1	2	0.11
(1,1984)	1:310:A:PHE:H	1:476:A:PHE:HE1	14	0.11
(1,1982)	1:228:A:MET:HE1	1:476:A:PHE:HD1	5	0.11
(1,1982)	1:228:A:MET:HE2	1:476:A:PHE:HD1	5	0.11
(1,1982)	1:228:A:MET:HE3	1:476:A:PHE:HD1	5	0.11
(1,1955)	1:226:A:TYR:H	1:475:A:VAL:HB	17	0.11
(1,1953)	1:225:A:VAL:HG11	1:475:A:VAL:HB	16	0.11
(1,1953)	1:225:A:VAL:HG12	1:475:A:VAL:HB	16	0.11
(1,1953)	1:225:A:VAL:HG13	1:475:A:VAL:HB	16	0.11
(1,1953)	1:225:A:VAL:HG21	1:475:A:VAL:HB	16	0.11
(1,1953)	1:225:A:VAL:HG22	1:475:A:VAL:HB	16	0.11
(1,1953)	1:225:A:VAL:HG23	1:475:A:VAL:HB	16	0.11
(1,1944)	1:473:A:LYS:HA	1:474:A:LEU:HD11	17	0.11
(1,1944)	1:473:A:LYS:HA	1:474:A:LEU:HD12	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1944)	1:473:A:LYS:HA	1:474:A:LEU:HD13	17	0.11
(1,1942)	1:473:A:LYS:HE2	1:474:A:LEU:H	14	0.11
(1,1942)	1:473:A:LYS:HE3	1:474:A:LEU:H	14	0.11
(1,1933)	1:470:A:LEU:HD11	1:474:A:LEU:H	16	0.11
(1,1933)	1:470:A:LEU:HD12	1:474:A:LEU:H	16	0.11
(1,1933)	1:470:A:LEU:HD13	1:474:A:LEU:H	16	0.11
(1,1926)	1:400:A:LEU:HG	1:474:A:LEU:HD21	15	0.11
(1,1926)	1:400:A:LEU:HG	1:474:A:LEU:HD22	15	0.11
(1,1926)	1:400:A:LEU:HG	1:474:A:LEU:HD23	15	0.11
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD11	12	0.11
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD12	12	0.11
(1,1925)	1:399:A:PHE:HA	1:474:A:LEU:HD13	12	0.11
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD11	8	0.11
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD12	8	0.11
(1,1923)	1:353:A:LYS:H	1:474:A:LEU:HD13	8	0.11
(1,1892)	1:225:A:VAL:HB	1:473:A:LYS:HA	4	0.11
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD11	7	0.11
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD12	7	0.11
(1,1847)	1:401:A:LEU:H	1:470:A:LEU:HD13	7	0.11
(1,1845)	1:400:A:LEU:HA	1:470:A:LEU:HG	9	0.11
(1,1843)	1:399:A:PHE:H	1:470:A:LEU:HB2	12	0.11
(1,1843)	1:399:A:PHE:H	1:470:A:LEU:HB3	12	0.11
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG21	17	0.11
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG22	17	0.11
(1,1828)	1:468:A:PHE:HB3	1:469:A:THR:HG23	17	0.11
(1,1823)	1:400:A:LEU:HA	1:469:A:THR:H	16	0.11
(1,1817)	1:467:A:THR:HG21	1:468:A:PHE:H	5	0.11
(1,1817)	1:467:A:THR:HG22	1:468:A:PHE:H	5	0.11
(1,1817)	1:467:A:THR:HG23	1:468:A:PHE:H	5	0.11
(1,1806)	1:401:A:LEU:HB2	1:467:A:THR:HB	4	0.11
(1,1806)	1:401:A:LEU:HB3	1:467:A:THR:HB	4	0.11
(1,1798)	1:446:A:VAL:H	1:446:A:VAL:HB	13	0.11
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG21	11	0.11
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG22	11	0.11
(1,1773)	1:443:A:LEU:HG	1:444:A:THR:HG23	11	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD11	3	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD12	3	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD13	3	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD11	9	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD12	9	0.11
(1,1735)	1:439:A:ILE:H	1:442:A:ILE:HD13	9	0.11
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:435:A:ARG:H	1:436:A:GLY:HA3	11	0.11
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG2	20	0.11
(1,1657)	1:434:A:PRO:HB2	1:435:A:ARG:HG3	20	0.11
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG2	20	0.11
(1,1657)	1:434:A:PRO:HB3	1:435:A:ARG:HG3	20	0.11
(1,1648)	1:277:A:LEU:HD11	1:434:A:PRO:HA	10	0.11
(1,1648)	1:277:A:LEU:HD12	1:434:A:PRO:HA	10	0.11
(1,1648)	1:277:A:LEU:HD13	1:434:A:PRO:HA	10	0.11
(1,1648)	1:277:A:LEU:HD21	1:434:A:PRO:HA	10	0.11
(1,1648)	1:277:A:LEU:HD22	1:434:A:PRO:HA	10	0.11
(1,1648)	1:277:A:LEU:HD23	1:434:A:PRO:HA	10	0.11
(1,1610)	1:426:A:CYS:HA	1:430:A:ARG:H	8	0.11
(1,1587)	1:427:A:GLN:HB2	1:428:A:SER:H	18	0.11
(1,1587)	1:427:A:GLN:HB3	1:428:A:SER:H	18	0.11
(1,1578)	1:426:A:CYS:HB2	1:427:A:GLN:H	1	0.11
(1,1578)	1:426:A:CYS:HB3	1:427:A:GLN:H	1	0.11
(1,1565)	1:424:A:SER:HA	1:426:A:CYS:H	20	0.11
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB2	16	0.11
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB3	16	0.11
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB2	16	0.11
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB3	16	0.11
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB2	16	0.11
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB3	16	0.11
(1,1520)	1:415:A:PRO:HB2	1:416:A:ALA:H	4	0.11
(1,1520)	1:415:A:PRO:HB3	1:416:A:ALA:H	4	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD11	17	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD12	17	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD13	17	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD21	17	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD22	17	0.11
(1,1466)	1:355:A:PHE:H	1:400:A:LEU:HD23	17	0.11
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB1	8	0.11
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB2	8	0.11
(1,1443)	1:396:A:GLU:H	1:397:A:ALA:HB3	8	0.11
(1,1426)	1:393:A:ILE:HA	1:393:A:ILE:HD11	3	0.11
(1,1426)	1:393:A:ILE:HA	1:393:A:ILE:HD12	3	0.11
(1,1426)	1:393:A:ILE:HA	1:393:A:ILE:HD13	3	0.11
(1,1413)	1:390:A:THR:H	1:390:A:THR:HG21	5	0.11
(1,1413)	1:390:A:THR:H	1:390:A:THR:HG22	5	0.11
(1,1413)	1:390:A:THR:H	1:390:A:THR:HG23	5	0.11
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	18	0.11
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:380:A:TYR:HA	1:381:A:LEU:HG	7	0.11
(1,1367)	1:380:A:TYR:H	1:381:A:LEU:HA	6	0.11
(1,1355)	1:373:A:THR:HB	1:381:A:LEU:H	7	0.11
(1,1338)	1:373:A:THR:HB	1:380:A:TYR:HA	17	0.11
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB2	9	0.11
(1,1337)	1:373:A:THR:HB	1:380:A:TYR:HB3	9	0.11
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG2	13	0.11
(1,1327)	1:377:A:GLU:HA	1:377:A:GLU:HG3	13	0.11
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB2	9	0.11
(1,1317)	1:373:A:THR:HB	1:374:A:ASP:HB3	9	0.11
(1,1312)	1:248:A:ARG:HG2	1:373:A:THR:HB	9	0.11
(1,1312)	1:248:A:ARG:HG3	1:373:A:THR:HB	9	0.11
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	7	0.11
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	7	0.11
(1,1248)	1:357:A:ILE:HG21	1:358:A:GLN:H	17	0.11
(1,1248)	1:357:A:ILE:HG22	1:358:A:GLN:H	17	0.11
(1,1248)	1:357:A:ILE:HG23	1:358:A:GLN:H	17	0.11
(1,1236)	1:314:A:ILE:H	1:356:A:PHE:H	7	0.11
(1,1232)	1:311:A:ILE:HG21	1:356:A:PHE:HE1	15	0.11
(1,1232)	1:311:A:ILE:HG22	1:356:A:PHE:HE1	15	0.11
(1,1232)	1:311:A:ILE:HG23	1:356:A:PHE:HE1	15	0.11
(1,1224)	1:354:A:VAL:HG21	1:355:A:PHE:H	13	0.11
(1,1224)	1:354:A:VAL:HG22	1:355:A:PHE:H	13	0.11
(1,1224)	1:354:A:VAL:HG23	1:355:A:PHE:H	13	0.11
(1,1192)	1:349:A:ALA:HA	1:351:A:LYS:H	16	0.11
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	9	0.11
(1,1188)	1:348:A:LEU:H	1:350:A:GLY:H	10	0.11
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB1	18	0.11
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB2	18	0.11
(1,1182)	1:346:A:PRO:HB2	1:349:A:ALA:HB3	18	0.11
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB1	18	0.11
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB2	18	0.11
(1,1182)	1:346:A:PRO:HB3	1:349:A:ALA:HB3	18	0.11
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	5	0.11
(1,1163)	1:304:A:HIS:HD2	1:348:A:LEU:HG	20	0.11
(1,1154)	1:344:A:LYS:HG2	1:345:A:CYS:H	9	0.11
(1,1151)	1:342:A:GLY:HA2	1:345:A:CYS:H	7	0.11
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	7	0.11
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	9	0.11
(1,1147)	1:341:A:THR:HG21	1:345:A:CYS:H	2	0.11
(1,1147)	1:341:A:THR:HG22	1:345:A:CYS:H	2	0.11
(1,1147)	1:341:A:THR:HG23	1:345:A:CYS:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:343:A:LEU:HB2	1:344:A:LYS:H	15	0.11
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	17	0.11
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	17	0.11
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB2	18	0.11
(1,1123)	1:340:A:PHE:H	1:344:A:LYS:HB3	18	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD11	6	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD12	6	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD13	6	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD21	6	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD22	6	0.11
(1,1115)	1:342:A:GLY:HA3	1:343:A:LEU:HD23	6	0.11
(1,1102)	1:340:A:PHE:HB2	1:341:A:THR:HA	6	0.11
(1,1102)	1:340:A:PHE:HB3	1:341:A:THR:HA	6	0.11
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	9	0.11
(1,1097)	1:339:A:GLN:H	1:341:A:THR:H	16	0.11
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB2	10	0.11
(1,1087)	1:337:A:THR:HA	1:339:A:GLN:HB3	10	0.11
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD11	1:337:A:THR:HG23	14	0.11
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD12	1:337:A:THR:HG23	14	0.11
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD13	1:337:A:THR:HG23	14	0.11
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD21	1:337:A:THR:HG23	14	0.11
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD22	1:337:A:THR:HG23	14	0.11
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG21	14	0.11
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG22	14	0.11
(1,1059)	1:296:A:LEU:HD23	1:337:A:THR:HG23	14	0.11
(1,1044)	1:335:A:GLU:H	1:336:A:LEU:HG	7	0.11
(1,1039)	1:334:A:TYR:H	1:336:A:LEU:HG	20	0.11
(1,1004)	1:332:A:PRO:HA	1:334:A:TYR:HB2	6	0.11
(1,997)	1:330:A:GLU:HA	1:331:A:ALA:H	7	0.11
(1,995)	1:293:A:TYR:HD1	1:331:A:ALA:HB1	6	0.11
(1,995)	1:293:A:TYR:HD1	1:331:A:ALA:HB2	6	0.11
(1,995)	1:293:A:TYR:HD1	1:331:A:ALA:HB3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE21	6	0.11
(1,979)	1:329:A:GLN:HA	1:329:A:GLN:HE22	6	0.11
(1,969)	1:325:A:GLY:H	1:329:A:GLN:H	14	0.11
(1,959)	1:326:A:THR:H	1:328:A:GLY:H	10	0.11
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA2	13	0.11
(1,953)	1:247:A:ALA:HA	1:328:A:GLY:HA3	13	0.11
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA2	10	0.11
(1,952)	1:246:A:LYS:HB2	1:328:A:GLY:HA3	10	0.11
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA2	10	0.11
(1,952)	1:246:A:LYS:HB3	1:328:A:GLY:HA3	10	0.11
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB2	9	0.11
(1,947)	1:288:A:THR:HG21	1:327:A:ASP:HB3	9	0.11
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB2	9	0.11
(1,947)	1:288:A:THR:HG22	1:327:A:ASP:HB3	9	0.11
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB2	9	0.11
(1,947)	1:288:A:THR:HG23	1:327:A:ASP:HB3	9	0.11
(1,937)	1:326:A:THR:H	1:326:A:THR:HB	8	0.11
(1,936)	1:288:A:THR:HG21	1:326:A:THR:HG21	20	0.11
(1,936)	1:288:A:THR:HG21	1:326:A:THR:HG22	20	0.11
(1,936)	1:288:A:THR:HG21	1:326:A:THR:HG23	20	0.11
(1,936)	1:288:A:THR:HG22	1:326:A:THR:HG21	20	0.11
(1,936)	1:288:A:THR:HG22	1:326:A:THR:HG22	20	0.11
(1,936)	1:288:A:THR:HG22	1:326:A:THR:HG23	20	0.11
(1,936)	1:288:A:THR:HG23	1:326:A:THR:HG21	20	0.11
(1,936)	1:288:A:THR:HG23	1:326:A:THR:HG22	20	0.11
(1,936)	1:288:A:THR:HG23	1:326:A:THR:HG23	20	0.11
(1,933)	1:324:A:TYR:HB3	1:325:A:GLY:H	9	0.11
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG2	3	0.11
(1,876)	1:319:A:ASP:HA	1:320:A:LYS:HG3	3	0.11
(1,868)	1:316:A:SER:H	1:317:A:HIS:H	20	0.11
(1,828)	1:311:A:ILE:HD11	1:312:A:CYS:H	14	0.11
(1,828)	1:311:A:ILE:HD12	1:312:A:CYS:H	14	0.11
(1,828)	1:311:A:ILE:HD13	1:312:A:CYS:H	14	0.11
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	17	0.11
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	17	0.11
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	17	0.11
(1,803)	1:309:A:CYS:HB2	1:310:A:PHE:H	5	0.11
(1,803)	1:309:A:CYS:HB3	1:310:A:PHE:H	5	0.11
(1,799)	1:309:A:CYS:HB3	1:310:A:PHE:H	20	0.11
(1,796)	1:307:A:MET:HB2	1:309:A:CYS:H	16	0.11
(1,796)	1:307:A:MET:HB3	1:309:A:CYS:H	16	0.11
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE1	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE2	16	0.11
(1,784)	1:235:A:TYR:HE1	1:307:A:MET:HE3	16	0.11
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	2	0.11
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	2	0.11
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	4	0.11
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	4	0.11
(1,746)	1:299:A:TYR:HB2	1:302:A:MET:HG3	14	0.11
(1,746)	1:299:A:TYR:HB3	1:302:A:MET:HG3	14	0.11
(1,715)	1:299:A:TYR:HD1	1:300:A:GLN:H	14	0.11
(1,698)	1:298:A:ILE:HD11	1:299:A:TYR:H	18	0.11
(1,698)	1:298:A:ILE:HD12	1:299:A:TYR:H	18	0.11
(1,698)	1:298:A:ILE:HD13	1:299:A:TYR:H	18	0.11
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD2	15	0.11
(1,655)	1:295:A:ILE:HA	1:297:A:LYS:HD3	15	0.11
(1,569)	1:287:A:CYS:HB2	1:292:A:ILE:HD11	6	0.11
(1,569)	1:287:A:CYS:HB2	1:292:A:ILE:HD12	6	0.11
(1,569)	1:287:A:CYS:HB2	1:292:A:ILE:HD13	6	0.11
(1,569)	1:287:A:CYS:HB3	1:292:A:ILE:HD11	6	0.11
(1,569)	1:287:A:CYS:HB3	1:292:A:ILE:HD12	6	0.11
(1,569)	1:287:A:CYS:HB3	1:292:A:ILE:HD13	6	0.11
(1,539)	1:288:A:THR:HG21	1:290:A:GLU:H	17	0.11
(1,539)	1:288:A:THR:HG22	1:290:A:GLU:H	17	0.11
(1,539)	1:288:A:THR:HG23	1:290:A:GLU:H	17	0.11
(1,469)	1:280:A:GLU:HB3	1:281:A:ILE:HA	18	0.11
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD11	12	0.11
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD12	12	0.11
(1,468)	1:280:A:GLU:H	1:281:A:ILE:HD13	12	0.11
(1,448)	1:238:A:ILE:HD11	1:281:A:ILE:HA	12	0.11
(1,448)	1:238:A:ILE:HD12	1:281:A:ILE:HA	12	0.11
(1,448)	1:238:A:ILE:HD13	1:281:A:ILE:HA	12	0.11
(1,435)	1:235:A:TYR:HB2	1:280:A:GLU:HB3	18	0.11
(1,435)	1:235:A:TYR:HB3	1:280:A:GLU:HB3	18	0.11
(1,419)	1:233:A:ARG:H	1:279:A:PHE:HA	17	0.11
(1,413)	1:276:A:GLU:H	1:278:A:HIS:H	6	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD11	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD12	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD13	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD21	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD22	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD23	15	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD11	16	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD12	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD13	16	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD21	16	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD22	16	0.11
(1,402)	1:276:A:GLU:H	1:277:A:LEU:HD23	16	0.11
(1,355)	1:271:A:THR:HG21	1:274:A:PHE:HB2	7	0.11
(1,355)	1:271:A:THR:HG21	1:274:A:PHE:HB3	7	0.11
(1,355)	1:271:A:THR:HG22	1:274:A:PHE:HB2	7	0.11
(1,355)	1:271:A:THR:HG22	1:274:A:PHE:HB3	7	0.11
(1,355)	1:271:A:THR:HG23	1:274:A:PHE:HB2	7	0.11
(1,355)	1:271:A:THR:HG23	1:274:A:PHE:HB3	7	0.11
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	20	0.11
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	20	0.11
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	20	0.11
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	17	0.11
(1,284)	1:265:A:LEU:H	1:265:A:LEU:HG	14	0.11
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD11	12	0.11
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD12	12	0.11
(1,264)	1:257:A:ILE:HA	1:257:A:ILE:HD13	12	0.11
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG21	20	0.11
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG22	20	0.11
(1,251)	1:254:A:LEU:HB2	1:257:A:ILE:HG23	20	0.11
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG21	20	0.11
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG22	20	0.11
(1,251)	1:254:A:LEU:HB3	1:257:A:ILE:HG23	20	0.11
(1,241)	1:255:A:HIS:HA	1:255:A:HIS:HD2	1	0.11
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	1	0.11
(1,238)	1:254:A:LEU:HA	1:255:A:HIS:H	11	0.11
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD21	8	0.11
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD22	8	0.11
(1,229)	1:253:A:LYS:HE2	1:254:A:LEU:HD23	8	0.11
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD21	8	0.11
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD22	8	0.11
(1,229)	1:253:A:LYS:HE3	1:254:A:LEU:HD23	8	0.11
(1,226)	1:253:A:LYS:H	1:254:A:LEU:HD21	5	0.11
(1,226)	1:253:A:LYS:H	1:254:A:LEU:HD22	5	0.11
(1,226)	1:253:A:LYS:H	1:254:A:LEU:HD23	5	0.11
(1,216)	1:251:A:VAL:HB	1:254:A:LEU:HG	5	0.11
(1,186)	1:247:A:ALA:HA	1:251:A:VAL:H	2	0.11
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	7	0.11
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	7	0.11
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	7	0.11
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	7	0.11
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	7	0.11
(1,130)	1:244:A:PHE:HA	1:246:A:LYS:H	7	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD11	6	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD12	6	0.11
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD13	6	0.11
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	4	0.11
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	18	0.11
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	18	0.11
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB2	2	0.11
(1,20)	1:225:A:VAL:HB	1:226:A:TYR:HB3	2	0.11
(1,7)	1:224:A:LYS:HB3	1:225:A:VAL:HB	18	0.11
(1,2017)	1:277:A:LEU:HD11	1:479:A:ASP:H	15	0.1
(1,2017)	1:277:A:LEU:HD12	1:479:A:ASP:H	15	0.1
(1,2017)	1:277:A:LEU:HD13	1:479:A:ASP:H	15	0.1
(1,2017)	1:277:A:LEU:HD21	1:479:A:ASP:H	15	0.1
(1,2017)	1:277:A:LEU:HD22	1:479:A:ASP:H	15	0.1
(1,2017)	1:277:A:LEU:HD23	1:479:A:ASP:H	15	0.1
(1,1903)	1:438:A:ASP:HA	1:473:A:LYS:HG2	17	0.1
(1,1903)	1:438:A:ASP:HA	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG2	17	0.1
(1,1899)	1:225:A:VAL:HG11	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG12	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG13	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG21	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG22	1:473:A:LYS:HG3	17	0.1
(1,1899)	1:225:A:VAL:HG23	1:473:A:LYS:HG3	17	0.1
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE2	14	0.1
(1,1893)	1:225:A:VAL:HB	1:473:A:LYS:HE3	14	0.1
(1,1892)	1:225:A:VAL:HB	1:473:A:LYS:HA	6	0.1
(1,1854)	1:469:A:THR:HG21	1:470:A:LEU:H	10	0.1
(1,1854)	1:469:A:THR:HG22	1:470:A:LEU:H	10	0.1
(1,1854)	1:469:A:THR:HG23	1:470:A:LEU:H	10	0.1
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG21	5	0.1
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG22	5	0.1
(1,1829)	1:468:A:PHE:HA	1:469:A:THR:HG23	5	0.1
(1,1807)	1:443:A:LEU:HD11	1:467:A:THR:H	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1807)	1:443:A:LEU:HD12	1:467:A:THR:H	11	0.1
(1,1807)	1:443:A:LEU:HD13	1:467:A:THR:H	11	0.1
(1,1807)	1:443:A:LEU:HD21	1:467:A:THR:H	11	0.1
(1,1807)	1:443:A:LEU:HD22	1:467:A:THR:H	11	0.1
(1,1807)	1:443:A:LEU:HD23	1:467:A:THR:H	11	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD11	19	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD12	19	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD13	19	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD21	19	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD22	19	0.1
(1,1769)	1:443:A:LEU:HA	1:443:A:LEU:HD23	19	0.1
(1,1766)	1:443:A:LEU:HA	1:443:A:LEU:HG	6	0.1
(1,1667)	1:434:A:PRO:HA	1:436:A:GLY:H	5	0.1
(1,1659)	1:434:A:PRO:HD2	1:435:A:ARG:H	4	0.1
(1,1659)	1:434:A:PRO:HD3	1:435:A:ARG:H	4	0.1
(1,1643)	1:431:A:GLU:H	1:433:A:CYS:H	17	0.1
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB2	6	0.1
(1,1550)	1:422:A:ILE:HD11	1:425:A:LEU:HB3	6	0.1
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB2	6	0.1
(1,1550)	1:422:A:ILE:HD12	1:425:A:LEU:HB3	6	0.1
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB2	6	0.1
(1,1550)	1:422:A:ILE:HD13	1:425:A:LEU:HB3	6	0.1
(1,1527)	1:417:A:GLU:H	1:418:A:GLY:H	5	0.1
(1,1504)	1:357:A:ILE:HG12	1:403:A:MET:HE1	18	0.1
(1,1504)	1:357:A:ILE:HG12	1:403:A:MET:HE2	18	0.1
(1,1504)	1:357:A:ILE:HG12	1:403:A:MET:HE3	18	0.1
(1,1504)	1:357:A:ILE:HG13	1:403:A:MET:HE1	18	0.1
(1,1504)	1:357:A:ILE:HG13	1:403:A:MET:HE2	18	0.1
(1,1504)	1:357:A:ILE:HG13	1:403:A:MET:HE3	18	0.1
(1,1469)	1:399:A:PHE:H	1:400:A:LEU:H	7	0.1
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG21	13	0.1
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG22	13	0.1
(1,1412)	1:389:A:GLN:HE21	1:390:A:THR:HG23	13	0.1
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG21	13	0.1
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG22	13	0.1
(1,1412)	1:389:A:GLN:HE22	1:390:A:THR:HG23	13	0.1
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG2	20	0.1
(1,1392)	1:383:A:MET:HA	1:383:A:MET:HG3	20	0.1
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB2	7	0.1
(1,1345)	1:379:A:PRO:HB2	1:380:A:TYR:HB3	7	0.1
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB2	7	0.1
(1,1345)	1:379:A:PRO:HB3	1:380:A:TYR:HB3	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:248:A:ARG:HD2	1:376:A:GLU:HA	10	0.1
(1,1320)	1:248:A:ARG:HD3	1:376:A:GLU:HA	10	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	10	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	10	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	14	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	14	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG2	15	0.1
(1,1309)	1:372:A:GLU:HA	1:372:A:GLU:HG3	15	0.1
(1,1286)	1:369:A:ILE:HG13	1:370:A:PRO:HD2	2	0.1
(1,1286)	1:369:A:ILE:HG13	1:370:A:PRO:HD2	6	0.1
(1,1267)	1:360:A:ALA:HB1	1:361:A:GLN:HA	7	0.1
(1,1267)	1:360:A:ALA:HB2	1:361:A:GLN:HA	7	0.1
(1,1267)	1:360:A:ALA:HB3	1:361:A:GLN:HA	7	0.1
(1,1266)	1:360:A:ALA:HB1	1:361:A:GLN:HG2	1	0.1
(1,1266)	1:360:A:ALA:HB1	1:361:A:GLN:HG3	1	0.1
(1,1266)	1:360:A:ALA:HB2	1:361:A:GLN:HG2	1	0.1
(1,1266)	1:360:A:ALA:HB2	1:361:A:GLN:HG3	1	0.1
(1,1266)	1:360:A:ALA:HB3	1:361:A:GLN:HG2	1	0.1
(1,1266)	1:360:A:ALA:HB3	1:361:A:GLN:HG3	1	0.1
(1,1231)	1:311:A:ILE:HG21	1:356:A:PHE:HD1	17	0.1
(1,1231)	1:311:A:ILE:HG22	1:356:A:PHE:HD1	17	0.1
(1,1231)	1:311:A:ILE:HG23	1:356:A:PHE:HD1	17	0.1
(1,1150)	1:342:A:GLY:H	1:345:A:CYS:H	12	0.1
(1,1044)	1:335:A:GLU:H	1:336:A:LEU:HG	11	0.1
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB1	18	0.1
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB2	18	0.1
(1,992)	1:289:A:VAL:HB	1:331:A:ALA:HB3	18	0.1
(1,924)	1:323:A:ILE:H	1:324:A:TYR:H	3	0.1
(1,914)	1:322:A:ILE:H	1:323:A:ILE:H	3	0.1
(1,899)	1:320:A:LYS:HE2	1:322:A:ILE:H	14	0.1
(1,899)	1:320:A:LYS:HE3	1:322:A:ILE:H	14	0.1
(1,870)	1:317:A:HIS:HA	1:318:A:GLY:H	17	0.1
(1,860)	1:314:A:ILE:HG12	1:315:A:LEU:H	17	0.1
(1,860)	1:314:A:ILE:HG13	1:315:A:LEU:H	17	0.1
(1,809)	1:274:A:PHE:HB2	1:311:A:ILE:HD11	15	0.1
(1,809)	1:274:A:PHE:HB2	1:311:A:ILE:HD12	15	0.1
(1,809)	1:274:A:PHE:HB2	1:311:A:ILE:HD13	15	0.1
(1,809)	1:274:A:PHE:HB3	1:311:A:ILE:HD11	15	0.1
(1,809)	1:274:A:PHE:HB3	1:311:A:ILE:HD12	15	0.1
(1,809)	1:274:A:PHE:HB3	1:311:A:ILE:HD13	15	0.1
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD11	15	0.1
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD12	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:237:A:LEU:H	1:311:A:ILE:HD13	15	0.1
(1,801)	1:309:A:CYS:HB2	1:310:A:PHE:H	5	0.1
(1,762)	1:300:A:GLN:H	1:303:A:ASP:H	6	0.1
(1,744)	1:299:A:TYR:HB2	1:302:A:MET:HE1	14	0.1
(1,744)	1:299:A:TYR:HB2	1:302:A:MET:HE2	14	0.1
(1,744)	1:299:A:TYR:HB2	1:302:A:MET:HE3	14	0.1
(1,744)	1:299:A:TYR:HB3	1:302:A:MET:HE1	14	0.1
(1,744)	1:299:A:TYR:HB3	1:302:A:MET:HE2	14	0.1
(1,744)	1:299:A:TYR:HB3	1:302:A:MET:HE3	14	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD11	12	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD12	12	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD13	12	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD21	12	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD22	12	0.1
(1,727)	1:298:A:ILE:HG21	1:301:A:LEU:HD23	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD11	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD12	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD13	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD21	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD22	12	0.1
(1,727)	1:298:A:ILE:HG22	1:301:A:LEU:HD23	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD11	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD12	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD13	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD21	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD22	12	0.1
(1,727)	1:298:A:ILE:HG23	1:301:A:LEU:HD23	12	0.1
(1,697)	1:297:A:LYS:HA	1:299:A:TYR:H	2	0.1
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD11	8	0.1
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD12	8	0.1
(1,663)	1:294:A:GLU:HA	1:298:A:ILE:HD13	8	0.1
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD2	3	0.1
(1,661)	1:297:A:LYS:H	1:297:A:LYS:HD3	3	0.1
(1,653)	1:295:A:ILE:HG12	1:297:A:LYS:H	2	0.1
(1,653)	1:295:A:ILE:HG13	1:297:A:LYS:H	2	0.1
(1,644)	1:293:A:TYR:HE1	1:296:A:LEU:HG	3	0.1
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD11	19	0.1
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD12	19	0.1
(1,572)	1:288:A:THR:HA	1:292:A:ILE:HD13	19	0.1
(1,552)	1:288:A:THR:H	1:291:A:GLN:H	11	0.1
(1,494)	1:238:A:ILE:H	1:284:A:HIS:HD2	12	0.1
(1,485)	1:281:A:ILE:HG21	1:282:A:LYS:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:281:A:ILE:HG22	1:282:A:LYS:H	3	0.1
(1,485)	1:281:A:ILE:HG23	1:282:A:LYS:H	3	0.1
(1,461)	1:277:A:LEU:H	1:281:A:ILE:HD11	8	0.1
(1,461)	1:277:A:LEU:H	1:281:A:ILE:HD12	8	0.1
(1,461)	1:277:A:LEU:H	1:281:A:ILE:HD13	8	0.1
(1,357)	1:273:A:THR:HG21	1:274:A:PHE:H	19	0.1
(1,357)	1:273:A:THR:HG22	1:274:A:PHE:H	19	0.1
(1,357)	1:273:A:THR:HG23	1:274:A:PHE:H	19	0.1
(1,344)	1:269:A:ALA:HB1	1:273:A:THR:H	18	0.1
(1,344)	1:269:A:ALA:HB2	1:273:A:THR:H	18	0.1
(1,344)	1:269:A:ALA:HB3	1:273:A:THR:H	18	0.1
(1,343)	1:269:A:ALA:HA	1:273:A:THR:H	15	0.1
(1,300)	1:264:A:HIS:HA	1:267:A:ALA:HA	2	0.1
(1,288)	1:264:A:HIS:HA	1:266:A:ASP:H	9	0.1
(1,276)	1:258:A:ARG:H	1:259:A:ASP:HA	18	0.1
(1,263)	1:257:A:ILE:HG21	1:257:A:ILE:HD11	2	0.1
(1,263)	1:257:A:ILE:HG21	1:257:A:ILE:HD12	2	0.1
(1,263)	1:257:A:ILE:HG21	1:257:A:ILE:HD13	2	0.1
(1,263)	1:257:A:ILE:HG22	1:257:A:ILE:HD11	2	0.1
(1,263)	1:257:A:ILE:HG22	1:257:A:ILE:HD12	2	0.1
(1,263)	1:257:A:ILE:HG22	1:257:A:ILE:HD13	2	0.1
(1,263)	1:257:A:ILE:HG23	1:257:A:ILE:HD11	2	0.1
(1,263)	1:257:A:ILE:HG23	1:257:A:ILE:HD12	2	0.1
(1,263)	1:257:A:ILE:HG23	1:257:A:ILE:HD13	2	0.1
(1,260)	1:257:A:ILE:H	1:257:A:ILE:HB	7	0.1
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD2	9	0.1
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD3	9	0.1
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD2	20	0.1
(1,206)	1:253:A:LYS:HA	1:253:A:LYS:HD3	20	0.1
(1,173)	1:249:A:GLU:H	1:250:A:LYS:HA	11	0.1
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB2	13	0.1
(1,170)	1:247:A:ALA:HB1	1:250:A:LYS:HB3	13	0.1
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB2	13	0.1
(1,170)	1:247:A:ALA:HB2	1:250:A:LYS:HB3	13	0.1
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB2	13	0.1
(1,170)	1:247:A:ALA:HB3	1:250:A:LYS:HB3	13	0.1
(1,127)	1:244:A:PHE:HA	1:245:A:ALA:H	3	0.1
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD11	2	0.1
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD12	2	0.1
(1,95)	1:238:A:ILE:HB	1:238:A:ILE:HD13	2	0.1
(1,78)	1:235:A:TYR:HD1	1:236:A:CYS:H	1	0.1
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG2	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:231:A:LYS:H	1:231:A:LYS:HG3	17	0.1
(1,12)	1:225:A:VAL:H	1:225:A:VAL:HG21	4	0.1
(1,12)	1:225:A:VAL:H	1:225:A:VAL:HG22	4	0.1
(1,12)	1:225:A:VAL:H	1:225:A:VAL:HG23	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found