



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:35 PM UTC

PDB ID : 8K2S / pdb_00008k2s
BMRB ID : 36581
Title : The structure of HtpG M domain in complex with unstructured D131D binding site a
Authors : Qu, X.; Huang, C.
Deposited on : 2023-07-13

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

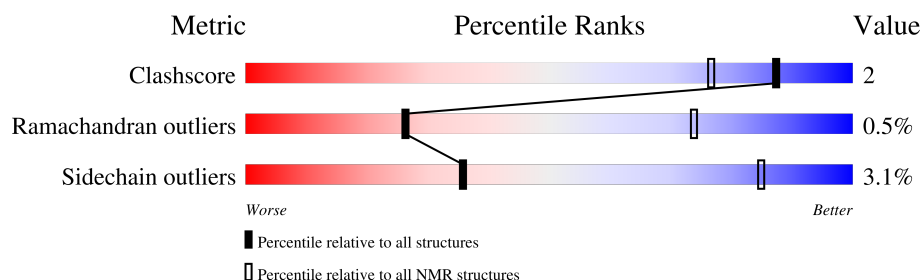
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 25%.

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	292	
2	B	77	

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:232-A:482, B:625-B:630 (257)	0.88	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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5302 atoms, of which 2643 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Molecular chaperone HtpG (Fragment).

Mol	Chain	Residues	Atoms						Trace
1	A	265	Total	C	H	N	O	S	0
			4333	1390	2146	371	419	7	

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MET	-	initiating methionine	UNP A0A7A6VTW3
A	204	LYS	-	expression tag	UNP A0A7A6VTW3
A	205	HIS	-	expression tag	UNP A0A7A6VTW3
A	206	HIS	-	expression tag	UNP A0A7A6VTW3
A	207	HIS	-	expression tag	UNP A0A7A6VTW3
A	208	HIS	-	expression tag	UNP A0A7A6VTW3
A	209	HIS	-	expression tag	UNP A0A7A6VTW3
A	210	HIS	-	expression tag	UNP A0A7A6VTW3
A	211	PRO	-	expression tag	UNP A0A7A6VTW3
A	212	MET	-	expression tag	UNP A0A7A6VTW3
A	213	SER	-	expression tag	UNP A0A7A6VTW3
A	214	ASP	-	expression tag	UNP A0A7A6VTW3
A	215	TYR	-	expression tag	UNP A0A7A6VTW3
A	216	ASP	-	expression tag	UNP A0A7A6VTW3
A	217	ILE	-	expression tag	UNP A0A7A6VTW3
A	218	PRO	-	expression tag	UNP A0A7A6VTW3
A	219	THR	-	expression tag	UNP A0A7A6VTW3
A	220	THR	-	expression tag	UNP A0A7A6VTW3
A	221	GLU	-	expression tag	UNP A0A7A6VTW3
A	222	ASN	-	expression tag	UNP A0A7A6VTW3
A	223	LEU	-	expression tag	UNP A0A7A6VTW3
A	224	TYR	-	expression tag	UNP A0A7A6VTW3
A	225	PHE	-	expression tag	UNP A0A7A6VTW3
A	226	GLN	-	expression tag	UNP A0A7A6VTW3
A	227	GLY	-	expression tag	UNP A0A7A6VTW3
A	228	HIS	-	expression tag	UNP A0A7A6VTW3
A	229	MET	-	expression tag	UNP A0A7A6VTW3

- Molecule 2 is a protein called Disordered protein (D131D).

Mol	Chain	Residues	Atoms						Trace
2	B	61	Total	C	H	N	O	S	0
			969	302	497	77	89	4	

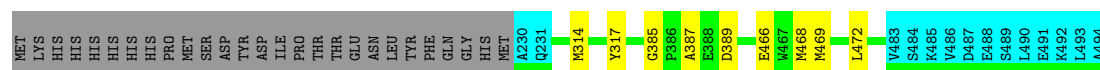
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

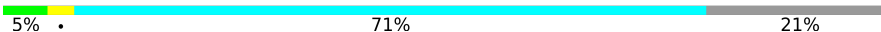
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

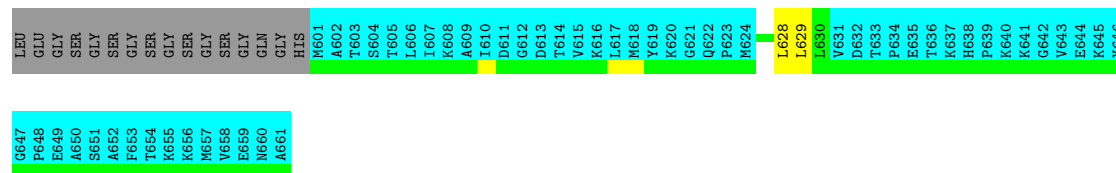
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 



- Molecule 2: Disordered protein (D131D)

Chain B: 



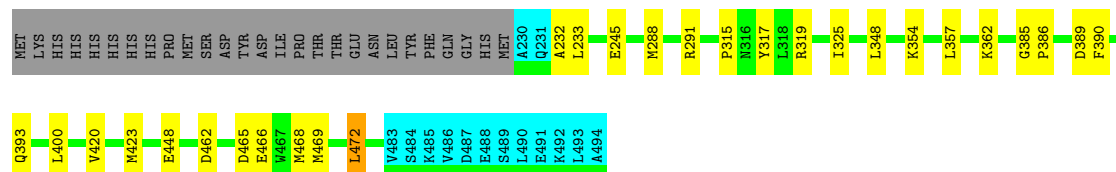
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

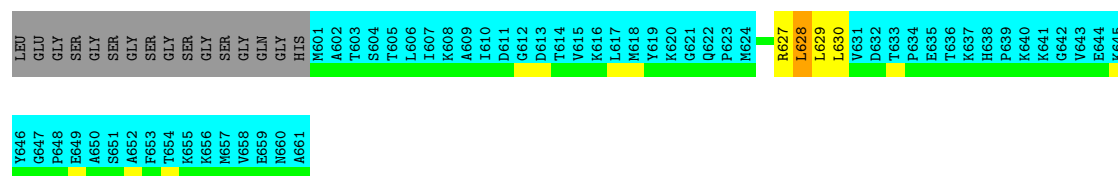
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 



- Molecule 2: Disordered protein (D131D)

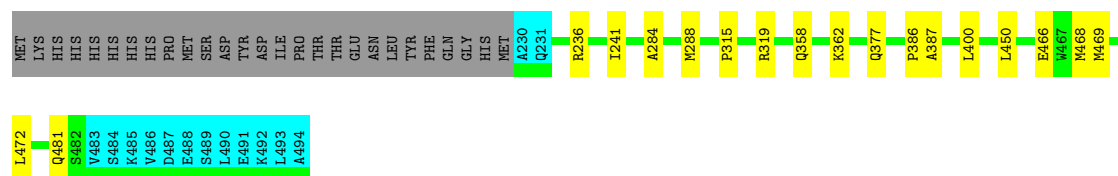
Chain B:  71% 21%



4.2.2 Score per residue for model 2

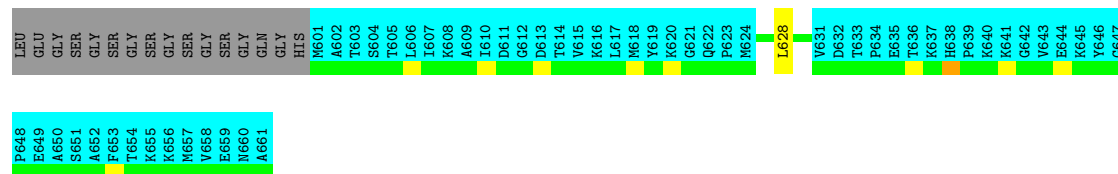
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:  80% 6% 5% 9%



- Molecule 2: Disordered protein (D131D)

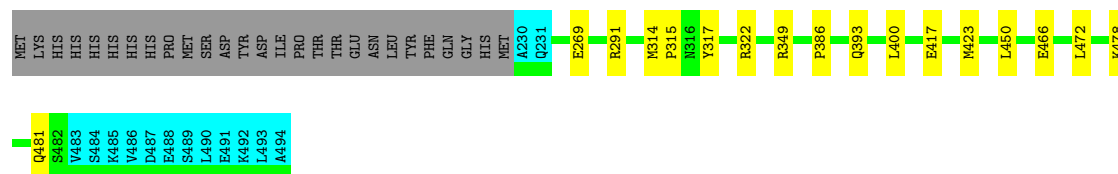
Chain B:  6% 71% 21%



4.2.3 Score per residue for model 3

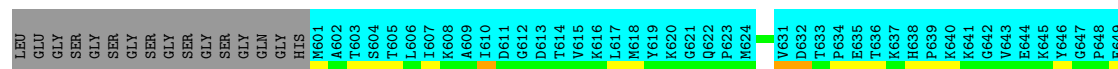
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:  80% 6% 5% 9%



- Molecule 2: Disordered protein (D131D)

Chain B:  8% 71% 21%

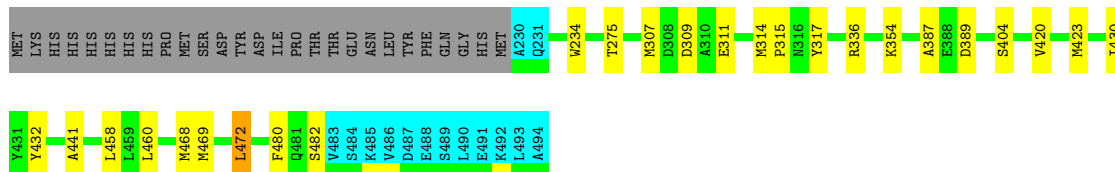




4.2.4 Score per residue for model 4

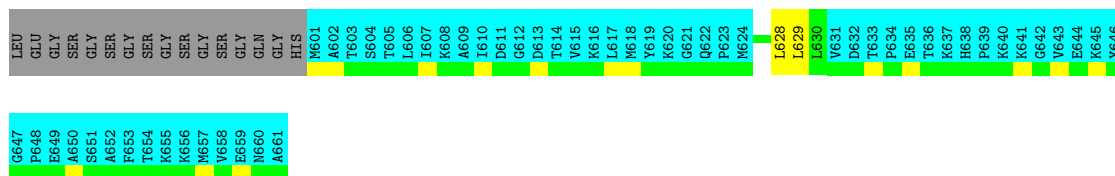
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 77% 8% 5% 9%



- Molecule 2: Disordered protein (D131D)

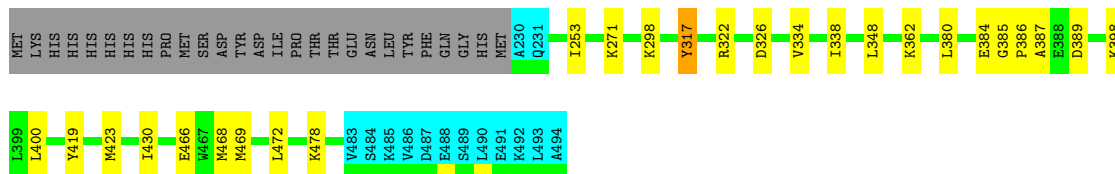
Chain B: 5% 71% 21%



4.2.5 Score per residue for model 5

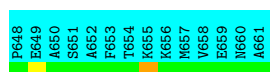
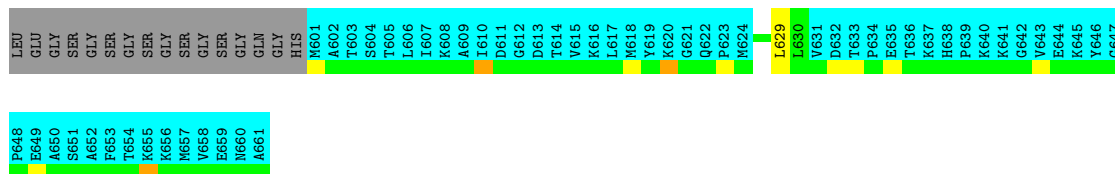
- Molecule 1: Molecular chaperone HtpG (Fragment)

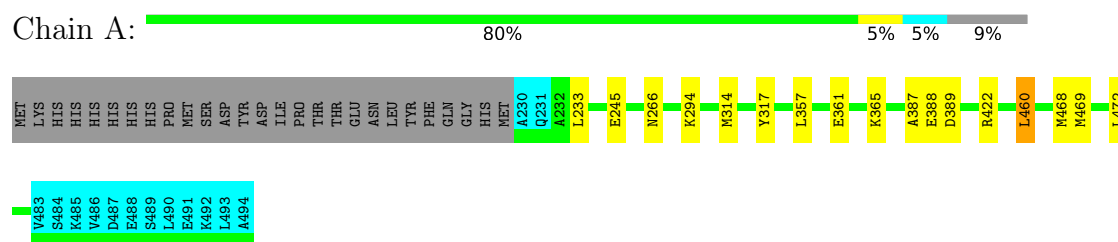
Chain A: 77% 9% 5% 9%



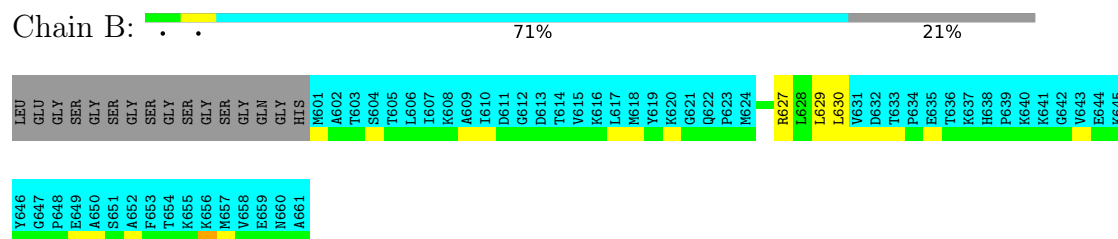
- Molecule 2: Disordered protein (D131D)

Chain B: 6% 71% 21%



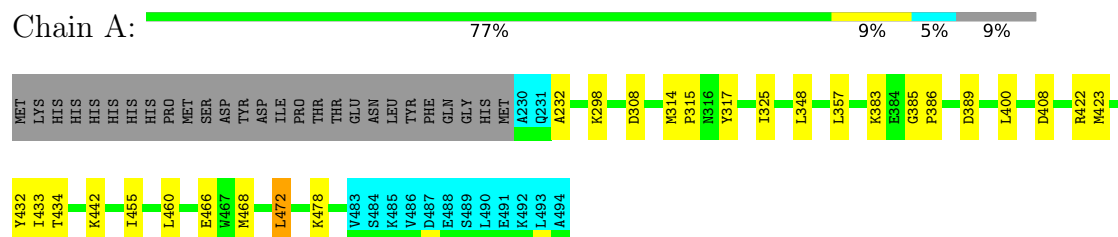


- Molecule 2: Disordered protein (D131D)

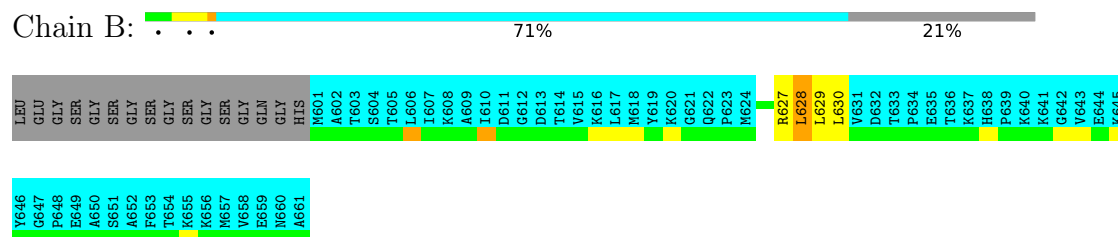


4.2.9 Score per residue for model 9

- Molecule 1: Molecular chaperone HtpG (Fragment)

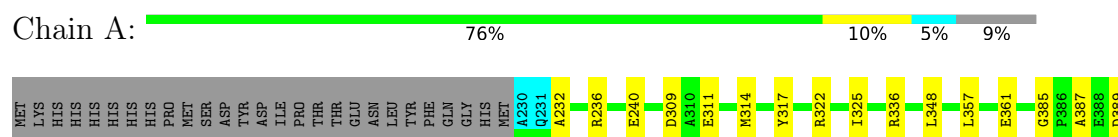


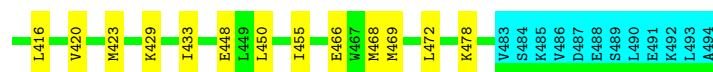
- Molecule 2: Disordered protein (D131D)



4.2.10 Score per residue for model 10

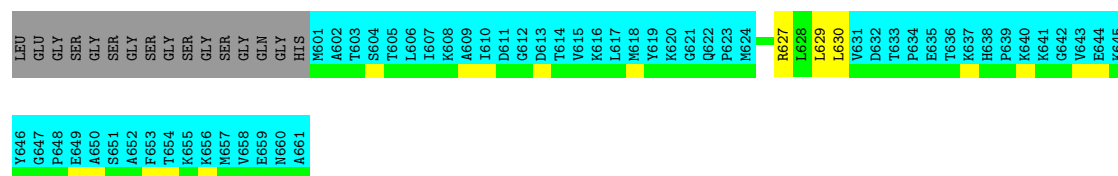
- Molecule 1: Molecular chaperone HtpG (Fragment)





- Molecule 2: Disordered protein (D131D)

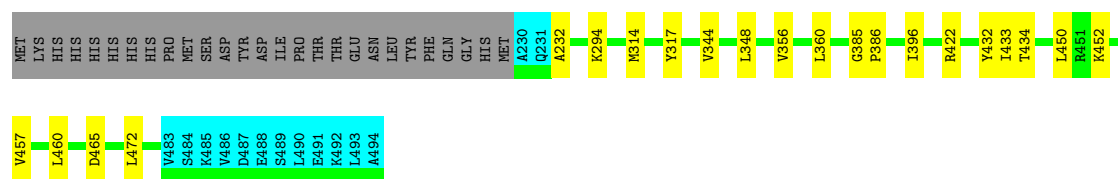
Chain B: . . 71% 21%



4.2.11 Score per residue for model 11

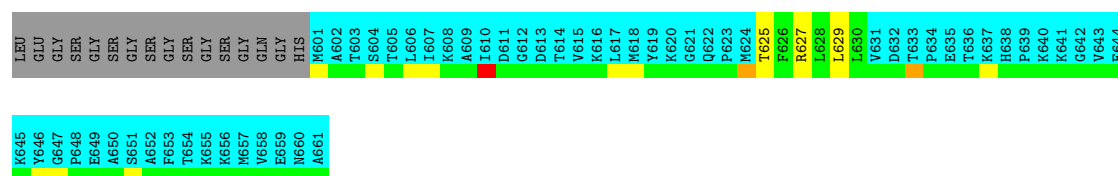
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 79% 7% 5% 9%



- Molecule 2: Disordered protein (D131D)

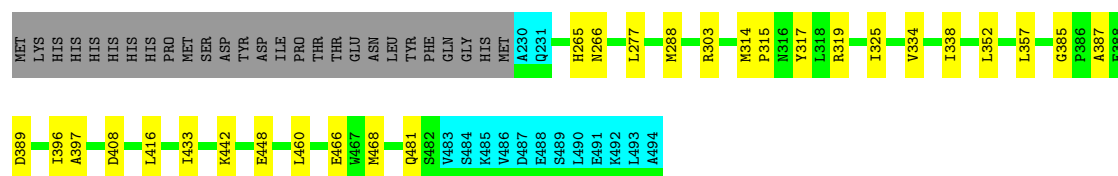
Chain B: . . 71% 21%



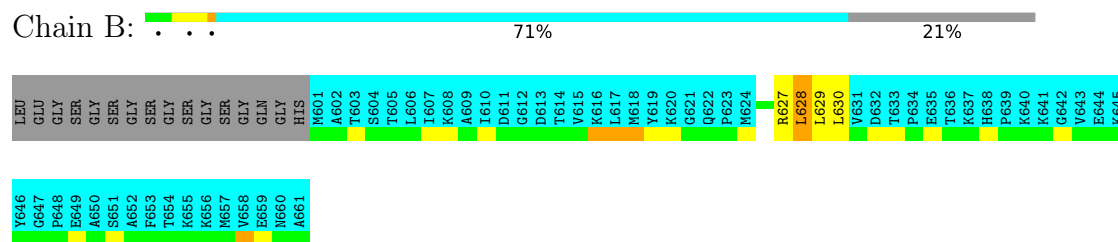
4.2.12 Score per residue for model 12

- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 76% 10% 5% 9%

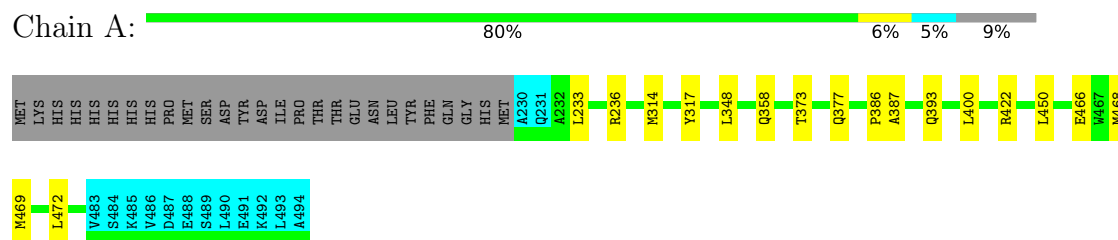


- Molecule 2: Disordered protein (D131D)

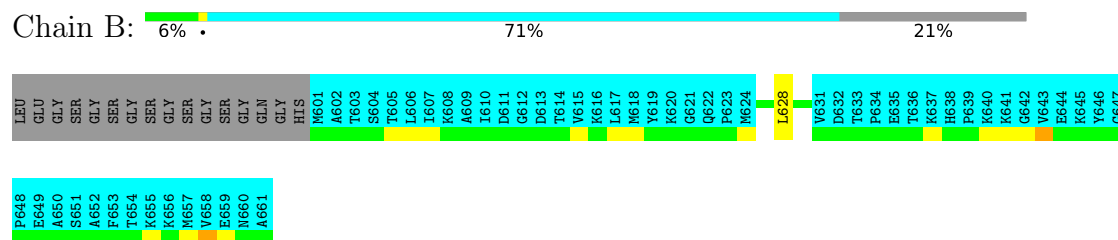


4.2.13 Score per residue for model 13

- Molecule 1: Molecular chaperone HtpG (Fragment)

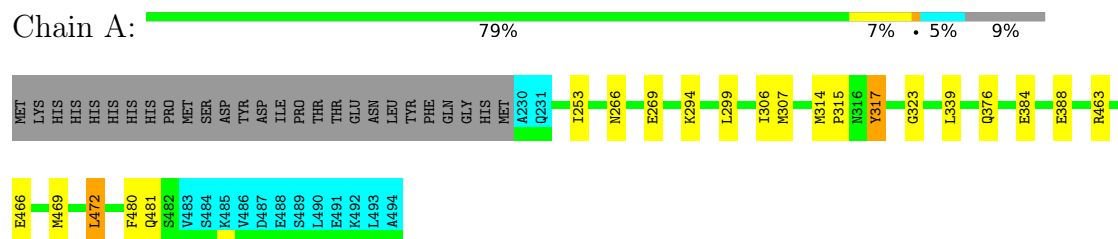


- Molecule 2: Disordered protein (D131D)

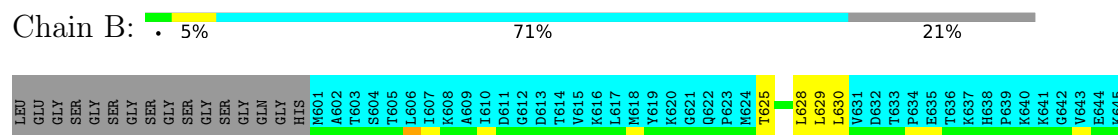


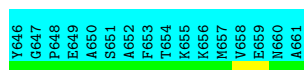
4.2.14 Score per residue for model 14

- Molecule 1: Molecular chaperone HtpG (Fragment)



- Molecule 2: Disordered protein (D131D)

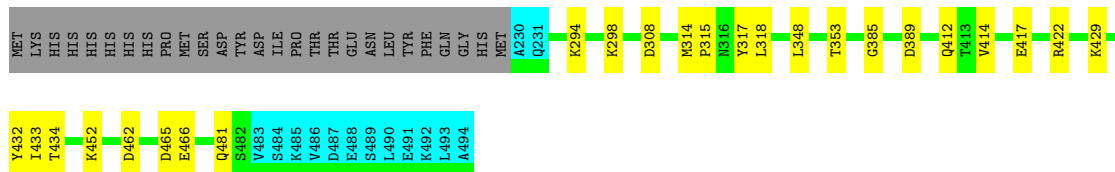




4.2.15 Score per residue for model 15

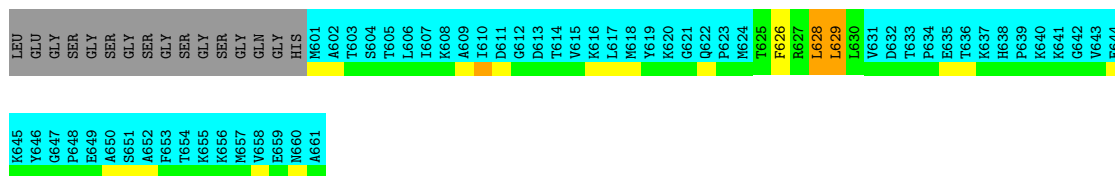
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 78% 8% 5% 9%



- Molecule 2: Disordered protein (D131D)

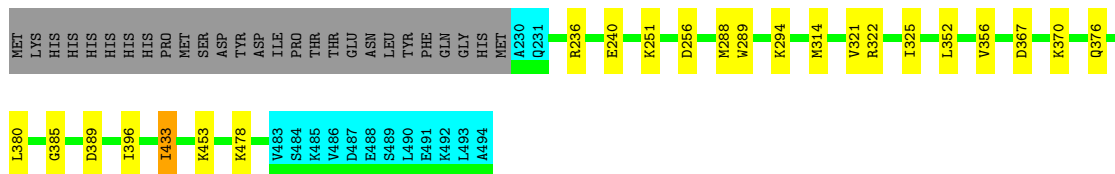
Chain B: 71% 21%



4.2.16 Score per residue for model 16

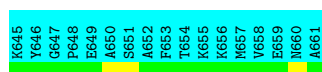
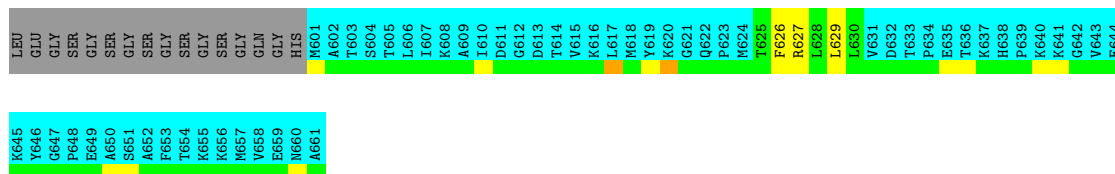
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 78% 8% 5% 9%



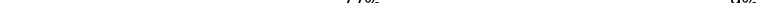
- Molecule 2: Disordered protein (D131D)

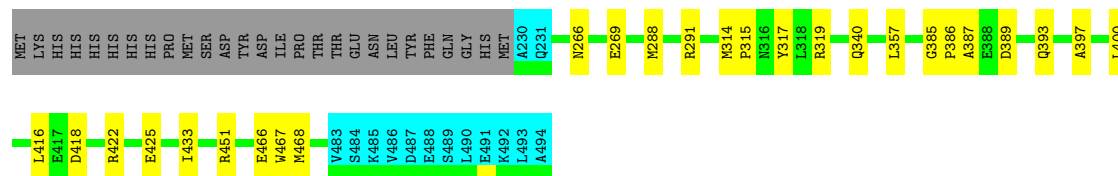
Chain B: 71% 21%



4.2.17 Score per residue for model 17

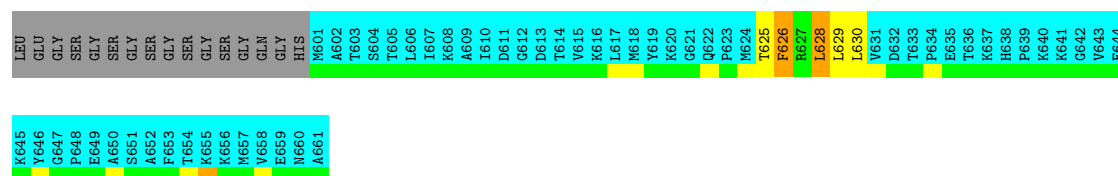
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:  77% 9% 5% 9%



- Molecule 2: Disordered protein (D131D)

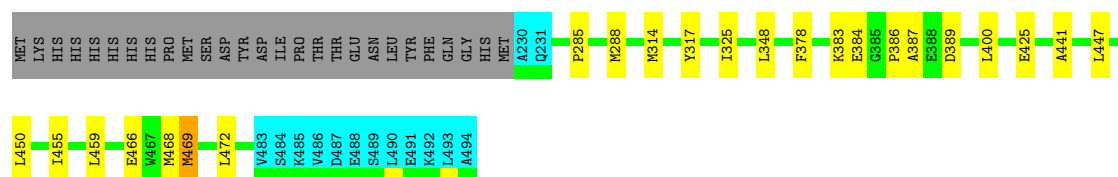
Chain B: 71% 21%



4.2.18 Score per residue for model 18

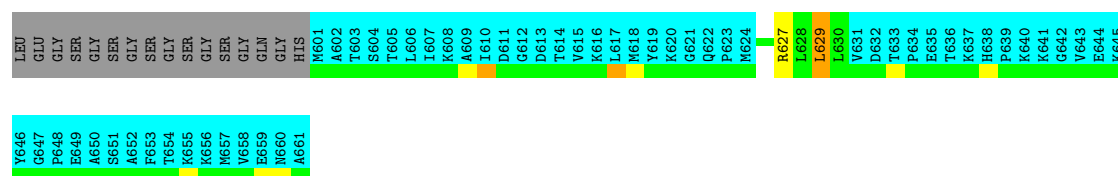
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 78% 8% 5% 9%



- Molecule 2: Disordered protein (D131D)

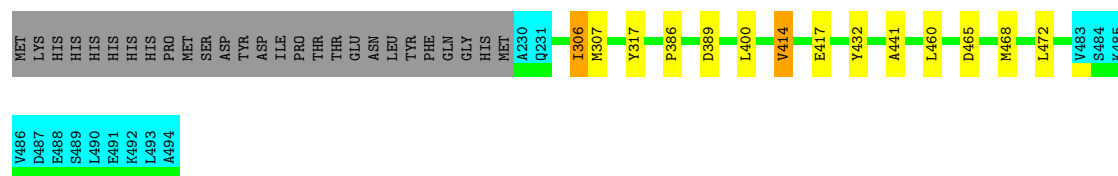
Chain B: 5% .. 71% 21%



4.2.19 Score per residue for model 19

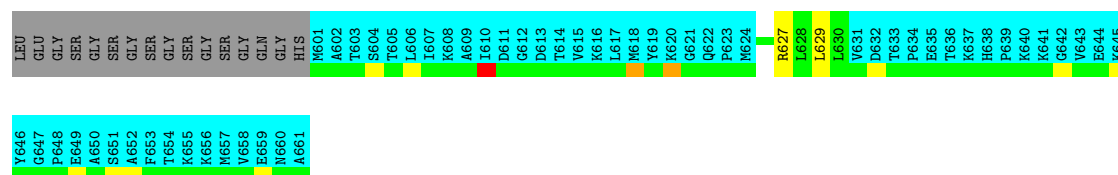
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 



- Molecule 2: Disordered protein (D131D)

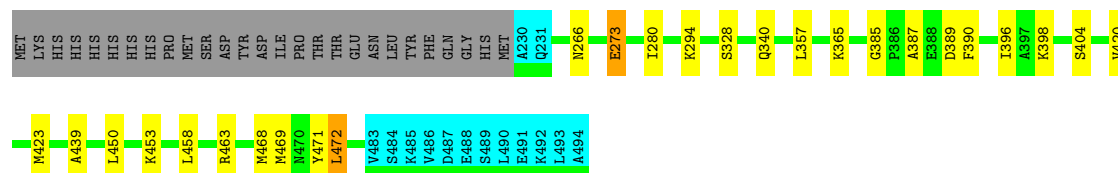
Chain B: 



4.2.20 Score per residue for model 20

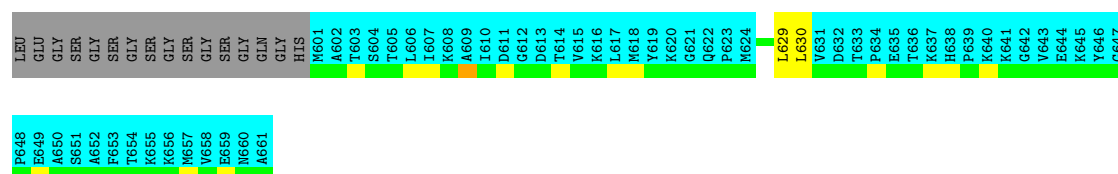
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A: 



- Molecule 2: Disordered protein (D131D)

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 100 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
CNS	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.15±0.02	0±0/2131 (0.0± 0.0%)	0.95±0.02	0±0/2882 (0.0± 0.0%)
2	B	1.44±0.11	0±0/54 (0.2± 0.6%)	1.06±0.11	0±0/73 (0.0± 0.0%)
All	All	1.16	5/43700 (0.0%)	0.96	2/59100 (0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	626	PHE	CA-C	6.35	1.56	1.52	17	2
1	A	414	VAL	CA-CB	5.65	1.60	1.54	19	1
1	A	280	ILE	CA-CB	5.46	1.59	1.54	20	1
1	A	306	ILE	CA-CB	5.09	1.60	1.55	19	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	406	HIS	CA-CB-CG	5.07	118.87	113.80	7	1
1	A	294	LYS	N-CA-C	-5.02	108.43	114.75	15	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2081	2036	2029	8±3
2	B	53	62	62	2±2
All	All	42680	41960	41820	167

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:389:ASP:HB3	2:B:629:LEU:HD12	0.64	1.67	10	14
1:A:462:ASP:HB2	1:A:465:ASP:HB2	0.61	1.73	1	1
1:A:387:ALA:HB2	1:A:468:MET:HA	0.59	1.73	5	12
1:A:317:TYR:HB3	1:A:384:GLU:HB2	0.58	1.75	5	3
1:A:462:ASP:HB3	1:A:465:ASP:HB2	0.57	1.75	15	1
1:A:357:LEU:HD12	2:B:630:LEU:HB3	0.56	1.77	9	4
1:A:469:MET:SD	1:A:472:LEU:HD23	0.54	2.42	10	1
1:A:319:ARG:NH1	1:A:381:VAL:HG13	0.53	2.19	7	1
1:A:306:ILE:HG22	1:A:307:MET:HG2	0.53	1.80	19	1
1:A:314:MET:SD	1:A:321:VAL:HB	0.53	2.44	16	1
1:A:253:ILE:HB	1:A:298:LYS:HD2	0.52	1.80	5	1
1:A:468:MET:SD	1:A:472:LEU:HD12	0.52	2.44	9	2
1:A:325:ILE:HG21	1:A:352:LEU:HD21	0.52	1.79	12	1
1:A:386:PRO:HG3	1:A:400:LEU:HD11	0.52	1.81	13	4
1:A:315:PRO:HG3	2:B:628:LEU:HD22	0.51	1.82	2	9
1:A:467:TRP:CH2	2:B:625:THR:HG21	0.51	2.41	17	1
1:A:288:MET:SD	1:A:319:ARG:HG3	0.50	2.45	2	3
1:A:390:PHE:HB3	1:A:471:TYR:HB3	0.50	1.82	20	1
1:A:469:MET:HA	1:A:472:LEU:HB2	0.50	1.83	14	4
1:A:390:PHE:HA	1:A:393:GLN:HB3	0.50	1.83	1	1
1:A:385:GLY:O	2:B:629:LEU:HD11	0.50	2.07	9	10
1:A:357:LEU:HB2	2:B:630:LEU:HD22	0.49	1.84	1	2
1:A:397:ALA:HB1	1:A:416:LEU:HD12	0.49	1.84	12	2
1:A:357:LEU:HD23	2:B:630:LEU:HD13	0.49	1.84	1	1
1:A:253:ILE:HD13	1:A:323:GLY:HA2	0.49	1.84	14	1
1:A:432:TYR:HB3	1:A:460:LEU:HD11	0.49	1.83	11	1
1:A:383:LYS:HE2	1:A:468:MET:SD	0.49	2.47	18	1
1:A:357:LEU:HB3	2:B:630:LEU:HD22	0.49	1.85	10	2
1:A:420:VAL:HA	1:A:423:MET:SD	0.48	2.48	4	3
1:A:298:LYS:HG2	1:A:308:ASP:HB3	0.48	1.86	15	1
1:A:423:MET:SD	1:A:478:LYS:HD3	0.48	2.48	3	1
1:A:298:LYS:HG2	1:A:308:ASP:HB2	0.48	1.84	9	1
1:A:386:PRO:HD3	1:A:396:ILE:HG21	0.48	1.86	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:ARG:HE	1:A:241:ILE:HG12	0.48	1.69	2	1
1:A:325:ILE:HD11	1:A:348:LEU:HD12	0.48	1.86	10	1
1:A:469:MET:SD	1:A:472:LEU:O	0.48	2.72	20	1
1:A:432:TYR:HD2	1:A:460:LEU:HD11	0.47	1.68	19	2
1:A:414:VAL:HG23	1:A:422:ARG:HH22	0.47	1.70	15	1
1:A:416:LEU:HD11	1:A:472:LEU:HD21	0.46	1.86	10	1
1:A:420:VAL:HA	1:A:423:MET:HG2	0.46	1.87	10	1
1:A:289:TRP:CH2	1:A:380:LEU:HB2	0.46	2.45	16	1
1:A:469:MET:SD	1:A:472:LEU:HB3	0.45	2.51	1	1
1:A:291:ARG:H	1:A:291:ARG:HD3	0.45	1.70	17	1
1:A:388:GLU:HB3	2:B:629:LEU:HD11	0.45	1.88	8	1
1:A:357:LEU:HD13	2:B:630:LEU:HD13	0.45	1.88	12	1
1:A:233:LEU:HA	1:A:236:ARG:HD3	0.45	1.87	13	1
1:A:386:PRO:HG2	1:A:468:MET:HG3	0.45	1.88	19	1
1:A:408:ASP:HB2	1:A:442:LYS:HE2	0.45	1.89	12	2
1:A:396:ILE:HD13	2:B:629:LEU:HD13	0.44	1.87	16	1
1:A:404:SER:HB3	1:A:458:LEU:HD23	0.44	1.89	4	2
1:A:234:TRP:O	1:A:275:THR:HG21	0.44	2.13	4	1
1:A:356:VAL:O	1:A:360:LEU:HG	0.44	2.13	11	1
1:A:236:ARG:NH2	1:A:240:GLU:HB3	0.44	2.27	16	2
1:A:450:LEU:HD13	1:A:457:VAL:HG21	0.44	1.90	11	1
1:A:314:MET:HA	1:A:314:MET:HE2	0.43	1.90	17	1
1:A:447:LEU:HD13	1:A:459:LEU:HD11	0.43	1.89	18	1
1:A:291:ARG:HD2	1:A:291:ARG:H	0.43	1.74	3	1
1:A:450:LEU:HB3	1:A:455:ILE:HG23	0.43	1.89	18	1
1:A:386:PRO:HG2	1:A:400:LEU:HD11	0.43	1.91	5	5
1:A:307:MET:HE1	1:A:336:ARG:HB2	0.43	1.90	4	1
1:A:358:GLN:O	1:A:362:LYS:HB2	0.43	2.14	2	1
1:A:389:ASP:O	2:B:629:LEU:HD12	0.43	2.14	16	1
1:A:418:ASP:O	1:A:422:ARG:HG2	0.43	2.14	17	1
1:A:396:ILE:HG12	2:B:630:LEU:HD12	0.43	1.90	20	1
1:A:334:VAL:HA	1:A:338:ILE:HD12	0.42	1.91	5	2
1:A:472:LEU:HB3	1:A:480:PHE:CE2	0.42	2.50	14	1
1:A:414:VAL:HG23	1:A:422:ARG:NH2	0.42	2.29	15	1
1:A:285:PRO:HG2	1:A:288:MET:HB2	0.42	1.91	18	1
1:A:423:MET:HE1	1:A:478:LYS:HG2	0.42	1.91	9	2
1:A:288:MET:HE1	1:A:378:PHE:HD2	0.42	1.75	18	1
1:A:273:GLU:HG2	1:A:328:SER:HB2	0.42	1.92	20	1
1:A:357:LEU:HG	2:B:630:LEU:HD13	0.42	1.90	20	1
1:A:251:LYS:HA	1:A:256:ASP:O	0.42	2.14	16	1
1:A:385:GLY:HA3	1:A:396:ILE:HG21	0.42	1.91	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:379:GLY:O	1:A:383:LYS:HG3	0.41	2.15	6	1
1:A:233:LEU:HD11	1:A:245:GLU:HB3	0.41	1.91	1	3
1:A:367:ASP:HB2	1:A:370:LYS:HE2	0.41	1.92	16	1
1:A:361:GLU:O	1:A:365:LYS:HG2	0.41	2.16	8	1
1:A:319:ARG:HH11	1:A:381:VAL:HG13	0.41	1.75	7	1
1:A:419:TYR:O	1:A:423:MET:HG3	0.41	2.15	7	1
1:A:318:LEU:HD11	1:A:353:THR:HG23	0.41	1.92	15	1
1:A:450:LEU:HD22	1:A:455:ILE:HD12	0.41	1.92	7	2
1:A:373:THR:O	1:A:377:GLN:HG2	0.41	2.16	13	1
1:A:344:VAL:O	1:A:348:LEU:HD23	0.41	2.15	11	1
1:A:265:HIS:HB2	1:A:277:LEU:HD13	0.41	1.92	12	1
1:A:306:ILE:HG22	1:A:307:MET:HG3	0.41	1.93	14	1
1:A:352:LEU:O	1:A:356:VAL:HG23	0.41	2.16	16	1
1:A:430:ILE:HD12	1:A:480:PHE:HE1	0.40	1.75	4	1
1:A:441:ALA:O	1:A:447:LEU:HD11	0.40	2.17	18	1
1:A:419:TYR:CE2	1:A:430:ILE:HG23	0.40	2.52	5	1
1:A:299:LEU:HD22	1:A:339:LEU:HD11	0.40	1.93	14	1
1:A:284:ALA:HB2	1:A:377:GLN:HB3	0.40	1.93	2	1
1:A:315:PRO:HG3	1:A:349:ARG:HE	0.40	1.77	3	1
1:A:469:MET:HE3	1:A:480:PHE:HB3	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	251/292 (86%)	242±2 (96±1%)	9±2 (3±1%)	0±0 (0±0%)	49	83
2	B	6/77 (8%)	3±1 (47±15%)	2±1 (35±12%)	1±1 (18±14%)	0	3
All	All	5140/7380 (70%)	4895 (95%)	217 (4%)	28 (1%)	26	74

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	627	ARG	9

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Mol	Chain	Res	Type	Models (Total)
2	B	628	LEU	7
1	A	232	ALA	4
2	B	629	LEU	3
1	A	472	LEU	2
2	B	630	LEU	2
2	B	625	THR	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	226/264 (86%)	219±2 (97±1%)	7±2 (3±1%)	35	84
2	B	6/61 (10%)	6±0 (98±5%)	0±0 (2±5%)	52	92
All	All	4640/6500 (71%)	4495 (97%)	145 (3%)	36	85

All 51 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	317	TYR	16
1	A	314	MET	12
1	A	472	LEU	10
1	A	348	LEU	7
1	A	325	ILE	5
1	A	481	GLN	5
1	A	294	LYS	5
1	A	269	GLU	4
1	A	322	ARG	4
1	A	393	GLN	4
1	A	417	GLU	4
1	A	266	ASN	4
1	A	422	ARG	4
1	A	448	GLU	3
1	A	309	ASP	3
1	A	311	GLU	3
1	A	398	LYS	3
1	A	433	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	291	ARG	2
1	A	354	LYS	2
1	A	362	LYS	2
1	A	429	LYS	2
1	A	478	LYS	2
1	A	452	LYS	2
1	A	288	MET	2
1	A	376	GLN	2
1	A	463	ARG	2
2	B	626	PHE	2
1	A	453	LYS	2
1	A	340	GLN	2
1	A	425	GLU	2
1	A	271	LYS	1
1	A	326	ASP	1
1	A	380	LEU	1
1	A	355	ARG	1
1	A	319	ARG	1
1	A	382	LEU	1
1	A	460	LEU	1
1	A	383	LYS	1
1	A	466	GLU	1
1	A	336	ARG	1
1	A	361	GLU	1
1	A	303	ARG	1
1	A	388	GLU	1
1	A	412	GLN	1
1	A	432	TYR	1
1	A	451	ARG	1
1	A	469	MET	1
1	A	414	VAL	1
1	A	273	GLU	1
1	A	365	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 25% for the well-defined parts and 21% 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	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	255	-0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	246	0.94 ± 0.09	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	227	-0.03 ± 0.26	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 25%, i.e. 899 atoms were assigned a chemical shift out of a possible 3668. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	667/1277 (52%)	213/514 (41%)	241/514 (47%)	213/249 (86%)
Sidechain	232/2035 (11%)	0/1314 (0%)	232/635 (37%)	0/86 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/356 (0%)	0/172 (0%)	0/164 (0%)	0/20 (0%)
Overall	899/3668 (25%)	213/2000 (11%)	473/1313 (36%)	213/355 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 955 atoms were assigned a chemical shift out of a possible 4575. 0 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	709/1618 (44%)	227/652 (35%)	255/652 (39%)	227/314 (72%)
Sidechain	246/2565 (10%)	0/1659 (0%)	246/806 (31%)	0/100 (0%)
Aromatic	0/392 (0%)	0/189 (0%)	0/181 (0%)	0/22 (0%)
Overall	955/4575 (21%)	227/2500 (9%)	501/1639 (31%)	227/436 (52%)

7.1.4 Statistically unusual chemical shifts ⓘ

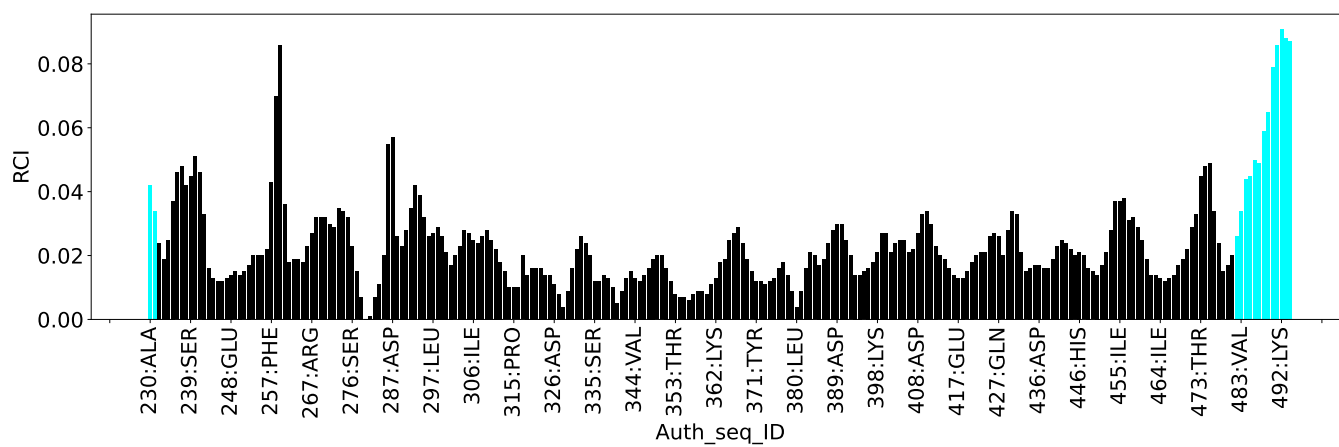
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	279	TYR	H	117.59	4.70 – 11.88	152.2
1	A	328	SER	H	31.14	5.45 – 11.10	40.5
1	A	340	GLN	H	29.41	5.39 – 11.05	37.5
1	A	279	TYR	N	9.63	100.12 – 140.79	-27.2
1	A	380	LEU	CB	57.53	33.11 – 51.34	8.4
1	A	335	SER	CB	51.64	56.28 – 71.32	-8.1
1	A	462	ASP	CB	53.22	32.98 – 48.76	7.8
1	A	380	LEU	CA	40.90	45.17 – 66.21	-7.0
1	A	360	LEU	CB	30.11	33.11 – 51.34	-6.7
1	A	353	THR	CB	58.99	61.12 – 78.27	-6.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3707
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	809
Medium range ($ i-j >1$ and $ i-j <5$)	1161
Long range ($ i-j \geq 5$)	1698
Inter-chain	37
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.0
Number of long range restraints per residue ¹	4.6

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)	50.1	0.2
0.2-0.5 (Medium)	98.3	0.5
>0.5 (Large)	5.0	3.63

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 ⓘ

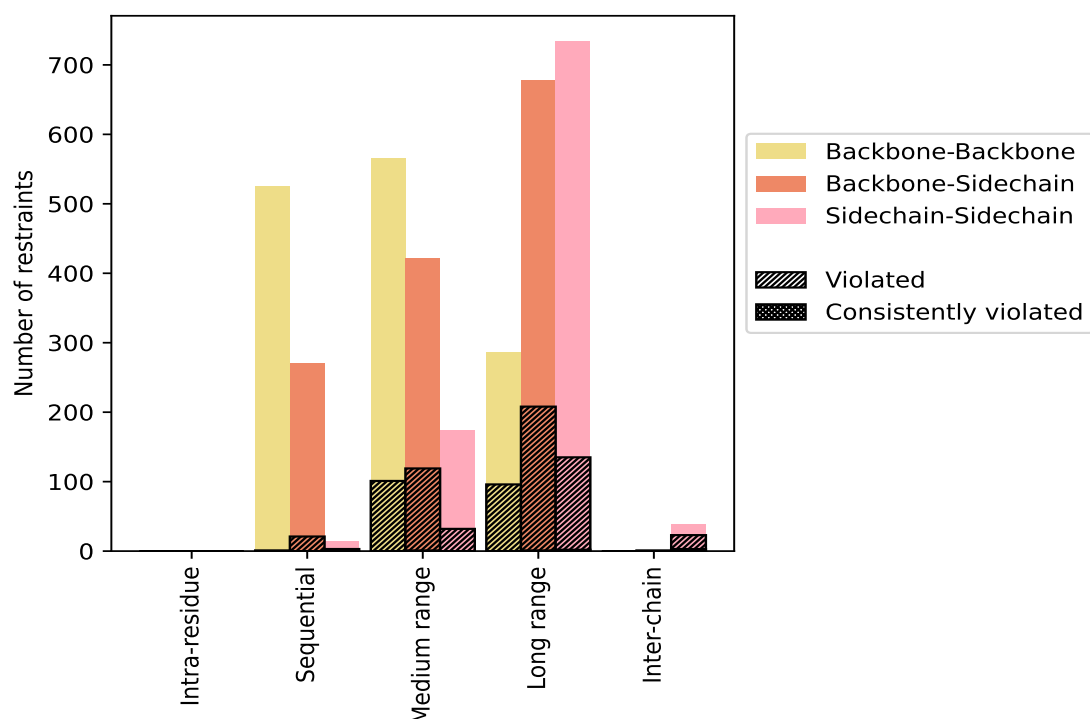
9.1 Summary of distance violations ⓘ

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)	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
Sequential (i-j =1)	809	21.8	25	3.1	0.7	0	0.0	0.0
Backbone-Backbone	525	14.2	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	270	7.3	21	7.8	0.6	0	0.0	0.0
Sidechain-Sidechain	14	0.4	3	21.4	0.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	1161	31.3	252	21.7	6.8	1	0.1	0.0
Backbone-Backbone	565	15.2	101	17.9	2.7	0	0.0	0.0
Backbone-Sidechain	422	11.4	119	28.2	3.2	1	0.2	0.0
Sidechain-Sidechain	174	4.7	32	18.4	0.9	0	0.0	0.0
Long range (i-j ≥5)	1698	45.8	439	25.9	11.8	3	0.2	0.1
Backbone-Backbone	286	7.7	96	33.6	2.6	0	0.0	0.0
Backbone-Sidechain	678	18.3	208	30.7	5.6	1	0.1	0.0
Sidechain-Sidechain	734	19.8	135	18.4	3.6	2	0.3	0.1
Inter-chain	37	1.0	22	59.5	0.6	3	8.1	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.0	1	100.0	0.0	0	0.0	0.0
Sidechain-Sidechain	36	1.0	21	58.3	0.6	3	8.3	0.1
Hydrogen bond	2	0.1	2	100.0	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3707	100.0	740	20.0	20.0	7	0.2	0.2
Backbone-Backbone	1376	37.1	198	14.4	5.3	0	0.0	0.0
Backbone-Sidechain	1371	37.0	349	25.5	9.4	2	0.1	0.1
Sidechain-Sidechain	960	25.9	193	20.1	5.2	5	0.5	0.1

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	0	4	41	105	12	162	0.25	0.75	0.12	0.23
2	0	9	46	107	9	171	0.26	0.75	0.11	0.26
3	0	3	43	101	13	160	0.28	2.66	0.22	0.26
4	0	5	64	75	13	157	0.28	2.05	0.17	0.26
5	0	8	54	88	15	165	0.25	0.79	0.12	0.24
6	0	8	41	90	12	151	0.28	2.4	0.2	0.26
7	0	5	47	97	13	162	0.27	1.58	0.15	0.25
8	0	5	58	76	11	150	0.26	0.58	0.1	0.26
9	0	7	54	76	14	151	0.29	2.71	0.26	0.26
10	0	5	54	87	11	157	0.25	0.75	0.11	0.24

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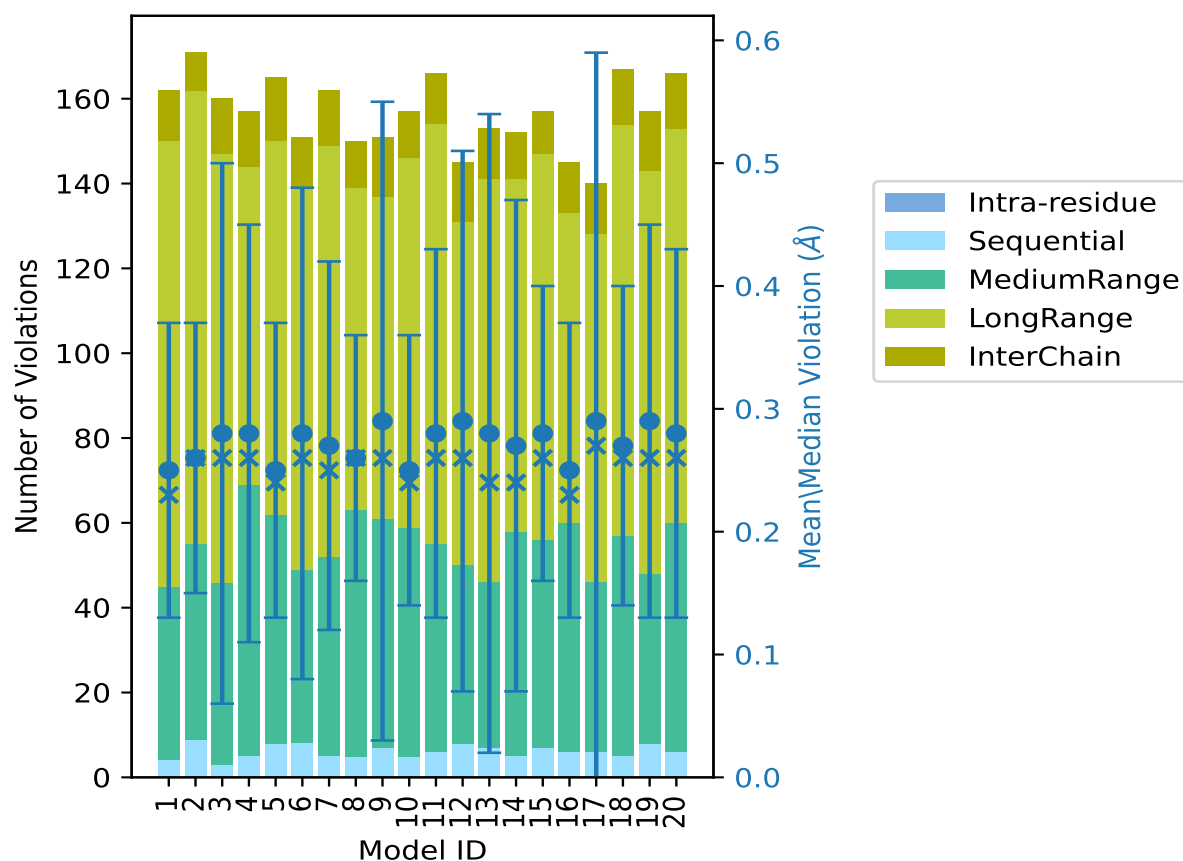
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	6	49	99	12	166	0.28	1.52	0.15	0.26
12	0	8	42	81	14	145	0.29	2.55	0.22	0.26
13	0	7	39	95	12	153	0.28	3.02	0.26	0.24
14	0	5	53	83	11	152	0.27	2.29	0.2	0.24
15	0	7	49	91	10	157	0.28	0.88	0.12	0.26
16	0	6	54	73	12	145	0.25	0.69	0.12	0.23
17	0	6	40	82	12	140	0.29	3.63	0.3	0.27
18	0	5	52	97	13	167	0.27	1.18	0.13	0.26
19	0	8	40	95	14	157	0.29	1.14	0.16	0.26
20	0	6	54	93	13	166	0.28	1.69	0.15	0.26

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

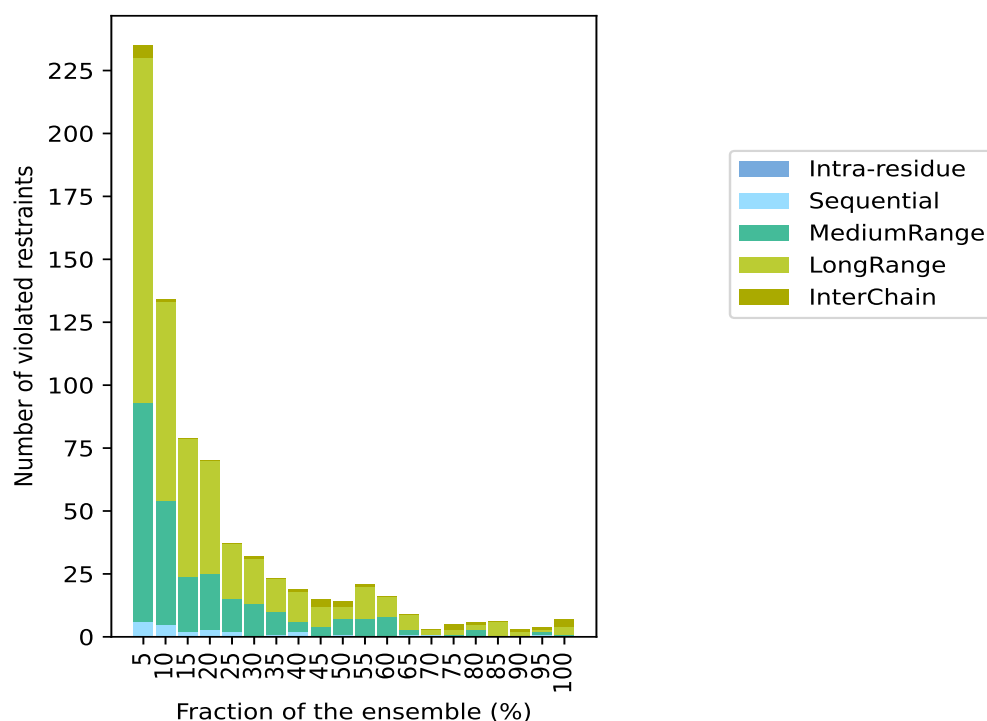
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2967(IR:0, SQ:784, MR:909, LR:1259, IC:15) restraints are 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	%
0	6	87	137	5	235	1	5.0
0	5	49	79	1	134	2	10.0
0	2	22	55	0	79	3	15.0
0	3	22	45	0	70	4	20.0
0	2	13	22	0	37	5	25.0
0	0	13	18	1	32	6	30.0
0	1	9	13	0	23	7	35.0
0	2	4	12	1	19	8	40.0
0	0	4	8	3	15	9	45.0
0	1	6	5	2	14	10	50.0
0	0	7	13	1	21	11	55.0
0	0	8	8	0	16	12	60.0
0	1	2	6	0	9	13	65.0
0	1	0	2	0	3	14	70.0
0	0	1	2	2	5	15	75.0
0	0	3	2	1	6	16	80.0
0	0	0	6	0	6	17	85.0
0	0	0	2	1	3	18	90.0
0	1	1	1	1	4	19	95.0
0	0	1	3	3	7	20	100.0

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

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

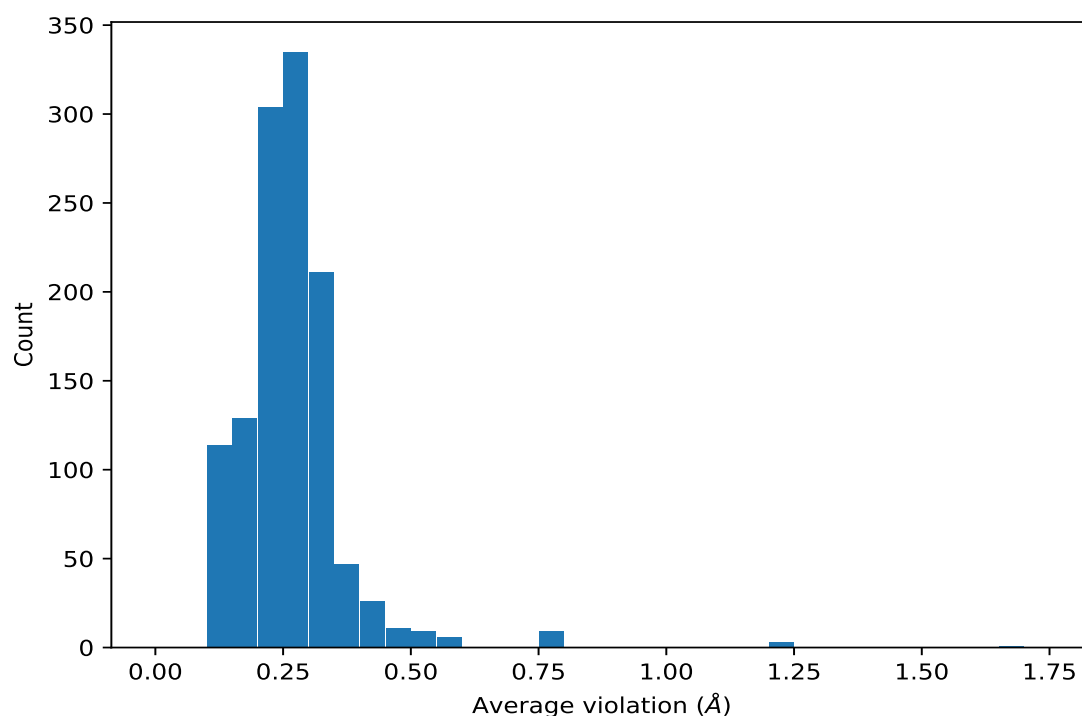
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	20	0.6	0.19	0.61
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	20	0.46	0.14	0.49
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	20	0.41	0.06	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	20	0.41	0.08	0.4
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	20	0.41	0.08	0.4
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	20	0.41	0.08	0.4
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	20	0.4	0.06	0.4
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	20	0.34	0.07	0.36
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	20	0.34	0.07	0.36
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	20	0.34	0.07	0.36
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	19	0.37	0.08	0.38
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	19	0.32	0.08	0.35
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	19	0.29	0.08	0.32
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	19	0.25	0.02	0.25
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	18	0.36	0.12	0.34
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	18	0.36	0.12	0.34
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	18	0.36	0.12	0.34
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	18	0.36	0.12	0.34
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	18	0.31	0.07	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	18	0.31	0.07	0.32
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	18	0.22	0.07	0.24
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	18	0.22	0.07	0.24
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	17	1.69	1.05	1.69
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	17	0.42	0.1	0.4
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	17	0.39	0.13	0.39
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	17	0.39	0.13	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	17	0.39	0.13	0.39
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	17	0.33	0.1	0.34
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	17	0.31	0.1	0.35
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	17	0.24	0.05	0.22
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	16	0.34	0.09	0.36
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	16	0.33	0.09	0.33
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	16	0.33	0.09	0.33
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	16	0.31	0.1	0.32
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	16	0.27	0.08	0.28
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	16	0.27	0.08	0.28
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	16	0.25	0.08	0.23
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	16	0.21	0.04	0.22
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	16	0.21	0.04	0.22
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	16	0.21	0.05	0.2
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	15	0.38	0.12	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	15	0.38	0.12	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	15	0.38	0.12	0.39
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	15	0.35	0.11	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	15	0.35	0.11	0.32
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	15	0.3	0.08	0.28
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	15	0.23	0.08	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	15	0.23	0.08	0.26
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	15	0.21	0.05	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	15	0.21	0.05	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	15	0.21	0.05	0.22
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	14	0.32	0.14	0.31
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	14	0.32	0.14	0.31
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	14	0.32	0.14	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	14	0.23	0.05	0.24
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	14	0.23	0.05	0.24
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	14	0.23	0.05	0.24
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	14	0.23	0.05	0.24
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	14	0.22	0.03	0.23
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	13	0.75	0.32	0.74
(1,3442)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	13	0.75	0.32	0.74
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	13	0.35	0.1	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	13	0.35	0.1	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	13	0.35	0.1	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	13	0.35	0.1	0.34
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	13	0.33	0.07	0.33
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	13	0.33	0.07	0.33
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	13	0.33	0.07	0.33
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	13	0.33	0.07	0.33
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	13	0.28	0.08	0.3
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	13	0.27	0.1	0.27
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	13	0.27	0.1	0.27
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	13	0.27	0.11	0.24
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	13	0.24	0.09	0.26
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	13	0.24	0.09	0.26
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	13	0.23	0.06	0.23
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	13	0.23	0.06	0.23
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	13	0.23	0.06	0.23
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	13	0.21	0.05	0.19
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	13	0.21	0.05	0.19
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	12	0.42	0.07	0.44
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	12	0.42	0.07	0.44
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	12	0.42	0.07	0.44
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	12	0.38	0.1	0.39
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	12	0.38	0.1	0.39
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	12	0.38	0.1	0.39
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	12	0.32	0.09	0.32
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	12	0.32	0.09	0.32
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	12	0.32	0.1	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	12	0.32	0.1	0.34
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	12	0.29	0.07	0.29
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	12	0.27	0.09	0.27
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	12	0.27	0.05	0.28
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	12	0.27	0.05	0.26
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	12	0.27	0.05	0.26
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	12	0.26	0.07	0.24
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	12	0.26	0.07	0.26
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	12	0.26	0.07	0.26
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	12	0.23	0.06	0.24
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	12	0.23	0.08	0.21
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	12	0.23	0.08	0.21
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	12	0.22	0.08	0.22
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	12	0.22	0.08	0.22
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	12	0.2	0.08	0.21
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	12	0.18	0.04	0.18
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	12	0.17	0.05	0.16
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	12	0.17	0.05	0.16
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	11	0.42	0.05	0.44
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	11	0.42	0.05	0.44
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	11	0.42	0.05	0.44
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	11	0.35	0.07	0.37
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	11	0.35	0.07	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	11	0.35	0.07	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	11	0.35	0.07	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	11	0.34	0.07	0.36
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	11	0.34	0.07	0.36
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	11	0.34	0.07	0.36
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	11	0.33	0.07	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	11	0.33	0.07	0.34
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	11	0.32	0.1	0.33
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	11	0.31	0.05	0.3
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	11	0.29	0.09	0.31
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	11	0.29	0.03	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	11	0.29	0.03	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	11	0.29	0.03	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	11	0.29	0.03	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	11	0.29	0.03	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	11	0.29	0.03	0.28
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	11	0.29	0.1	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	11	0.29	0.1	0.28
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	11	0.28	0.09	0.31
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	11	0.28	0.09	0.31
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	11	0.28	0.09	0.31
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	11	0.28	0.11	0.26
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	11	0.27	0.08	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	11	0.27	0.08	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	11	0.27	0.08	0.31
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	11	0.26	0.07	0.22
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	11	0.25	0.09	0.27
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	11	0.25	0.09	0.27
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	11	0.24	0.09	0.25
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	11	0.24	0.09	0.25
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	11	0.23	0.08	0.23
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	11	0.23	0.08	0.23
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	11	0.23	0.06	0.25
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	11	0.2	0.07	0.22
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	11	0.19	0.08	0.17
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	11	0.19	0.06	0.18
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	11	0.16	0.04	0.16
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	11	0.16	0.04	0.16
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	10	0.31	0.09	0.31
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	10	0.31	0.09	0.31
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	10	0.31	0.13	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	10	0.31	0.13	0.28
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	10	0.31	0.13	0.28
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	10	0.31	0.11	0.36
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	10	0.31	0.11	0.36
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	10	0.31	0.11	0.36
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	10	0.31	0.11	0.36
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	10	0.31	0.11	0.36
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	10	0.31	0.11	0.36
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	10	0.29	0.11	0.31
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	10	0.29	0.11	0.31
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	10	0.28	0.08	0.25
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	10	0.28	0.08	0.25
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	10	0.28	0.08	0.25
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	10	0.28	0.08	0.25
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	10	0.27	0.08	0.26
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	10	0.26	0.1	0.31
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	10	0.24	0.06	0.25
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	10	0.24	0.08	0.22
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	10	0.24	0.08	0.22
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	10	0.23	0.08	0.22
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	10	0.22	0.1	0.2
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	10	0.22	0.1	0.2
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	10	0.21	0.09	0.22
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	10	0.21	0.07	0.18
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	10	0.18	0.05	0.18
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	9	0.35	0.06	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	9	0.35	0.06	0.37
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	9	0.33	0.06	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	9	0.33	0.06	0.34
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	9	0.33	0.06	0.34
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	9	0.32	0.07	0.32
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	9	0.32	0.07	0.32
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	9	0.32	0.07	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	9	0.32	0.07	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	9	0.32	0.07	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	9	0.32	0.07	0.32
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	9	0.3	0.08	0.29
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	9	0.29	0.09	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	9	0.29	0.09	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	9	0.29	0.09	0.34
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	9	0.29	0.07	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	9	0.29	0.07	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	9	0.29	0.07	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	9	0.29	0.07	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	9	0.29	0.07	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	9	0.29	0.07	0.29
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	9	0.28	0.06	0.29
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	9	0.28	0.06	0.29
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	9	0.27	0.18	0.16
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	9	0.27	0.18	0.16
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	9	0.27	0.18	0.16
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	9	0.26	0.07	0.23
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	9	0.26	0.07	0.23
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	9	0.25	0.05	0.26
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	9	0.25	0.06	0.24
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	9	0.24	0.08	0.27
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	9	0.23	0.09	0.19
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	9	0.23	0.09	0.19
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	9	0.22	0.04	0.23
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	9	0.2	0.03	0.19
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	9	0.2	0.03	0.19
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	8	0.5	0.13	0.5
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	8	0.5	0.13	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	8	0.34	0.08	0.34
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	8	0.34	0.08	0.34
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	8	0.34	0.08	0.34
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	8	0.34	0.08	0.36
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	8	0.34	0.08	0.36
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	8	0.34	0.08	0.36
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	8	0.34	0.08	0.36
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	8	0.34	0.08	0.36
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	8	0.34	0.08	0.36
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	8	0.33	0.06	0.3
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	8	0.33	0.06	0.3
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	8	0.31	0.09	0.31
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	8	0.28	0.11	0.24
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	8	0.28	0.07	0.28
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	8	0.28	0.07	0.28
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	8	0.27	0.08	0.3
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	8	0.27	0.08	0.3
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	8	0.27	0.08	0.3
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	8	0.27	0.1	0.29
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	8	0.27	0.1	0.29
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	8	0.27	0.08	0.24
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	8	0.26	0.1	0.28
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	8	0.26	0.1	0.28
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	8	0.26	0.07	0.29
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	8	0.26	0.07	0.29
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	8	0.26	0.07	0.29
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	8	0.26	0.07	0.29
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	8	0.26	0.07	0.29
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	8	0.26	0.07	0.29
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	8	0.25	0.04	0.26
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	8	0.23	0.07	0.2
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	8	0.23	0.07	0.2
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	8	0.23	0.07	0.2
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	8	0.22	0.05	0.24
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	8	0.22	0.08	0.2
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	8	0.2	0.09	0.18
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	8	0.18	0.05	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	8	0.18	0.05	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	8	0.18	0.05	0.17
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	8	0.18	0.04	0.21
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	8	0.13	0.02	0.13
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	8	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	7	0.35	0.06	0.33
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	7	0.3	0.03	0.29
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	7	0.27	0.07	0.29
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	7	0.27	0.05	0.26
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	7	0.27	0.05	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	7	0.27	0.05	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	7	0.27	0.05	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	7	0.27	0.05	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	7	0.27	0.05	0.26
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	7	0.27	0.08	0.3
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	7	0.27	0.08	0.3
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	7	0.26	0.11	0.31
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	7	0.26	0.11	0.31
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	7	0.26	0.07	0.31
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	7	0.26	0.07	0.31
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	7	0.26	0.07	0.31
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	7	0.26	0.07	0.23
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	7	0.26	0.07	0.23
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	7	0.26	0.07	0.23
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	7	0.26	0.06	0.27
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	7	0.26	0.06	0.27
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	7	0.26	0.06	0.28
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	7	0.26	0.06	0.28
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD2	7	0.25	0.17	0.19
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HE2	7	0.25	0.17	0.19
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD1	7	0.25	0.17	0.19
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	7	0.25	0.08	0.25
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	7	0.25	0.09	0.29
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	7	0.22	0.07	0.2
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	7	0.22	0.05	0.23
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	7	0.22	0.05	0.23
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	7	0.22	0.05	0.23
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	7	0.22	0.08	0.21
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	7	0.22	0.04	0.2
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	7	0.22	0.04	0.2
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	7	0.22	0.08	0.2
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	7	0.2	0.06	0.24
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	7	0.2	0.06	0.24
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	7	0.2	0.06	0.24
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	7	0.2	0.07	0.19
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	7	0.19	0.05	0.19
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	7	0.19	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	7	0.19	0.04	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	7	0.19	0.04	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	7	0.19	0.04	0.21
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	7	0.15	0.03	0.15
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	7	0.15	0.03	0.15
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	6	0.52	0.16	0.45
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	6	0.52	0.16	0.45
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	6	0.38	0.11	0.35
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	6	0.38	0.11	0.35
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	6	0.38	0.11	0.35
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	6	0.38	0.11	0.35
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	6	0.31	0.15	0.3
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	6	0.31	0.07	0.3
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	6	0.31	0.07	0.3
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	6	0.31	0.07	0.3
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	6	0.28	0.03	0.28
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	6	0.28	0.03	0.28
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	6	0.28	0.03	0.28
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	6	0.28	0.03	0.28
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	6	0.28	0.09	0.24
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	6	0.28	0.09	0.24
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	6	0.28	0.05	0.27
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	6	0.28	0.05	0.27
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	6	0.27	0.12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	6	0.27	0.12	0.24
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	6	0.27	0.04	0.26
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	6	0.27	0.04	0.26
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	6	0.26	0.07	0.26
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	6	0.26	0.07	0.26
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	6	0.26	0.07	0.26
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	6	0.26	0.07	0.26
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	6	0.26	0.07	0.26
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	6	0.26	0.07	0.26
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	6	0.26	0.04	0.25
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	6	0.26	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	6	0.25	0.08	0.28
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	6	0.25	0.08	0.28
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	6	0.25	0.08	0.28
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	6	0.25	0.04	0.26
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	6	0.24	0.09	0.28
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	6	0.24	0.1	0.26
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	6	0.24	0.1	0.26
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	6	0.22	0.06	0.22
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	6	0.22	0.06	0.22
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	6	0.22	0.06	0.22
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	6	0.22	0.07	0.22
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	6	0.22	0.08	0.22
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	6	0.22	0.08	0.22
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	6	0.21	0.04	0.2
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	6	0.21	0.07	0.22
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	6	0.21	0.07	0.22
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	6	0.21	0.09	0.21
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	6	0.21	0.07	0.24
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	6	0.2	0.07	0.18
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	6	0.2	0.05	0.19
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	6	0.2	0.05	0.18
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	6	0.2	0.05	0.18
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	6	0.19	0.06	0.18
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	6	0.19	0.06	0.18
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	6	0.19	0.04	0.2
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	6	0.18	0.04	0.18
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	6	0.17	0.03	0.19
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	6	0.17	0.07	0.16
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	6	0.17	0.03	0.16
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	6	0.16	0.03	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	6	0.16	0.03	0.18
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	5	0.35	0.03	0.35
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	5	0.35	0.03	0.35
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	5	0.35	0.15	0.29
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	5	0.35	0.15	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	5	0.33	0.1	0.32
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	5	0.33	0.1	0.32
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	5	0.32	0.05	0.3
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	5	0.32	0.05	0.3
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	5	0.31	0.06	0.29
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	5	0.31	0.06	0.29
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	5	0.29	0.07	0.31
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	5	0.29	0.07	0.31
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	5	0.29	0.08	0.31
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	5	0.29	0.08	0.31
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	5	0.29	0.08	0.31
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	5	0.29	0.08	0.31
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	5	0.29	0.1	0.24
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	5	0.29	0.1	0.24
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	5	0.29	0.1	0.24
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	5	0.29	0.1	0.24
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	5	0.29	0.14	0.36
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	5	0.28	0.09	0.3
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	5	0.28	0.09	0.3
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	5	0.28	0.09	0.3
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	5	0.28	0.09	0.3
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	5	0.27	0.06	0.25
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	5	0.26	0.08	0.29
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	5	0.26	0.08	0.29
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	5	0.26	0.08	0.29
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	5	0.26	0.08	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	5	0.26	0.08	0.29
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	5	0.26	0.08	0.23
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	5	0.25	0.07	0.22
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	5	0.25	0.07	0.22
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	5	0.23	0.07	0.24
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	5	0.23	0.07	0.24
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	5	0.23	0.07	0.21
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	5	0.22	0.06	0.23
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	5	0.22	0.12	0.17
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	5	0.22	0.06	0.23
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	5	0.21	0.06	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	5	0.21	0.06	0.25
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	5	0.21	0.06	0.25
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	5	0.21	0.05	0.22
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	5	0.21	0.05	0.22
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	5	0.21	0.05	0.21
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	5	0.2	0.07	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	5	0.2	0.07	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	5	0.2	0.07	0.25
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	5	0.2	0.07	0.23
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	5	0.19	0.01	0.2
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	5	0.19	0.08	0.13
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	5	0.19	0.08	0.18
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	5	0.19	0.05	0.22
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	5	0.18	0.06	0.17
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	5	0.18	0.06	0.18
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	5	0.18	0.06	0.18
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	5	0.18	0.09	0.12
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	5	0.18	0.09	0.12
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	5	0.18	0.09	0.12
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	5	0.17	0.03	0.17
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	5	0.17	0.08	0.13
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	5	0.17	0.08	0.13
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	5	0.17	0.08	0.13
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	5	0.17	0.08	0.13
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	5	0.16	0.05	0.16
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	5	0.16	0.03	0.17
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	5	0.15	0.03	0.15
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	4	0.5	0.1	0.51
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	4	0.5	0.1	0.51
(1,1509)	1:315:A:PRO:HG2	1:319:A:ARG:H	4	0.45	0.06	0.44
(1,1509)	1:315:A:PRO:HG3	1:319:A:ARG:H	4	0.45	0.06	0.44
(1,3385)	1:450:A:LEU:HA	1:455:A:ILE:HB	4	0.38	0.06	0.38
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE1	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE2	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE3	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE1	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE2	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE3	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE1	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE2	4	0.38	0.22	0.29
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE3	4	0.38	0.22	0.29
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	4	0.36	0.04	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB2	4	0.36	0.03	0.36
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB3	4	0.36	0.03	0.36
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD11	4	0.35	0.11	0.36
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD12	4	0.35	0.11	0.36
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD13	4	0.35	0.11	0.36
(1,2369)	1:380:A:LEU:HD11	1:463:A:ARG:H	4	0.35	0.03	0.36
(1,2369)	1:380:A:LEU:HD12	1:463:A:ARG:H	4	0.35	0.03	0.36
(1,2369)	1:380:A:LEU:HD13	1:463:A:ARG:H	4	0.35	0.03	0.36
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	4	0.34	0.1	0.38
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	4	0.34	0.1	0.38
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	4	0.34	0.1	0.38
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	4	0.34	0.1	0.38
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	4	0.34	0.1	0.38
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	4	0.34	0.1	0.38
(1,2207)	1:371:A:TYR:HD2	1:375:A:TRP:H	4	0.33	0.15	0.34
(1,2207)	1:371:A:TYR:HD1	1:375:A:TRP:H	4	0.33	0.15	0.34
(1,3200)	1:434:A:THR:HA	1:461:A:SER:HA	4	0.32	0.09	0.32
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB2	4	0.32	0.11	0.34
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB3	4	0.32	0.11	0.34
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	4	0.32	0.02	0.31
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	4	0.32	0.02	0.31
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	4	0.31	0.14	0.32
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	4	0.31	0.14	0.32
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	4	0.31	0.14	0.32
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	4	0.31	0.14	0.32
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	4	0.3	0.03	0.3
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	4	0.3	0.03	0.3
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	4	0.3	0.03	0.3
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	4	0.3	0.03	0.3
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	4	0.3	0.02	0.29
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	4	0.3	0.02	0.29
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	4	0.3	0.05	0.32
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	4	0.3	0.05	0.32
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB2	4	0.29	0.09	0.26
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB3	4	0.29	0.09	0.26
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	4	0.29	0.04	0.29
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	4	0.29	0.04	0.29
(1,3469)	1:462:A:ASP:HB2	1:464:A:ILE:H	4	0.28	0.01	0.29
(1,3469)	1:462:A:ASP:HB3	1:464:A:ILE:H	4	0.28	0.01	0.29
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD2	4	0.28	0.1	0.29
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD3	4	0.28	0.1	0.29
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	4	0.28	0.05	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	4	0.28	0.05	0.26
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	4	0.28	0.07	0.29
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	4	0.28	0.07	0.29
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	4	0.28	0.07	0.29
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	4	0.28	0.07	0.29
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	4	0.28	0.07	0.29
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	4	0.28	0.07	0.29
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	4	0.27	0.04	0.27
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	4	0.27	0.04	0.27
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	4	0.27	0.04	0.27
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	4	0.27	0.04	0.27
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	4	0.27	0.04	0.27
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	4	0.27	0.04	0.27
(1,3022)	1:423:A:MET:HA	1:456:A:GLU:H	4	0.27	0.09	0.29
(1,2827)	1:407:A:THR:H	1:409:A:SER:H	4	0.26	0.02	0.26
(1,2712)	1:402:A:PHE:H	1:413:A:THR:H	4	0.26	0.09	0.3
(1,3030)	1:423:A:MET:HE1	1:428:A:GLU:H	4	0.25	0.09	0.28
(1,3030)	1:423:A:MET:HE2	1:428:A:GLU:H	4	0.25	0.09	0.28
(1,3030)	1:423:A:MET:HE3	1:428:A:GLU:H	4	0.25	0.09	0.28
(1,3075)	1:427:A:GLN:HG2	1:429:A:LYS:H	4	0.25	0.09	0.28
(1,3075)	1:427:A:GLN:HG3	1:429:A:LYS:H	4	0.25	0.09	0.28
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB2	4	0.25	0.09	0.28
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB3	4	0.25	0.09	0.28
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	4	0.24	0.11	0.2
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	4	0.24	0.11	0.2
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	4	0.24	0.11	0.2
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	4	0.24	0.11	0.2
(1,3525)	1:468:A:MET:HA	1:472:A:LEU:H	4	0.24	0.08	0.24
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	4	0.24	0.03	0.23
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	4	0.24	0.03	0.23
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	4	0.24	0.03	0.23
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	4	0.24	0.08	0.25
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	4	0.24	0.08	0.25
(1,1068)	1:295:A:HIS:HE1	1:316:A:ASN:HA	4	0.24	0.08	0.29
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	4	0.24	0.06	0.22
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	4	0.24	0.06	0.22
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB2	4	0.24	0.07	0.26
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB3	4	0.24	0.07	0.26
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB2	4	0.24	0.07	0.26
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB3	4	0.24	0.07	0.26
(1,2469)	1:385:A:GLY:HA2	1:389:A:ASP:H	4	0.24	0.08	0.2
(1,2469)	1:385:A:GLY:HA3	1:389:A:ASP:H	4	0.24	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD11	4	0.23	0.05	0.24
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD12	4	0.23	0.05	0.24
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD13	4	0.23	0.05	0.24
(1,1023)	1:289:A:TRP:HH2	1:381:A:VAL:HA	4	0.22	0.06	0.22
(1,2229)	1:372:A:GLN:HE21	1:376:A:GLN:H	4	0.22	0.06	0.25
(1,2229)	1:372:A:GLN:HE22	1:376:A:GLN:H	4	0.22	0.06	0.25
(1,2836)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	4	0.22	0.08	0.24
(1,3582)	1:474:A:GLU:H	1:480:A:PHE:H	4	0.22	0.03	0.22
(1,1533)	1:317:A:TYR:HB2	1:385:A:GLY:H	4	0.22	0.08	0.22
(1,1533)	1:317:A:TYR:HB3	1:385:A:GLY:H	4	0.22	0.08	0.22
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	4	0.22	0.07	0.24
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG11	4	0.22	0.03	0.22
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG12	4	0.22	0.03	0.22
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG13	4	0.22	0.03	0.22
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	4	0.22	0.04	0.22
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	4	0.22	0.04	0.22
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	4	0.22	0.04	0.22
(1,1323)	1:302:A:GLN:H	1:327:A:SER:H	4	0.22	0.07	0.22
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG2	4	0.22	0.01	0.22
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG3	4	0.22	0.01	0.22
(1,3220)	1:436:A:ASP:HA	1:463:A:ARG:HA	4	0.22	0.08	0.2
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	4	0.21	0.07	0.21
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	4	0.21	0.07	0.21
(1,2639)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	4	0.21	0.08	0.21
(1,2639)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	4	0.21	0.08	0.21
(1,1320)	1:302:A:GLN:HA	1:328:A:SER:HA	4	0.2	0.06	0.2
(1,3136)	1:431:A:TYR:HA	1:482:A:SER:HA	4	0.2	0.07	0.21
(1,3062)	1:426:A:GLY:HA2	1:428:A:GLU:HA	4	0.2	0.08	0.16
(1,3062)	1:426:A:GLY:HA3	1:428:A:GLU:HA	4	0.2	0.08	0.16
(1,3152)	1:431:A:TYR:HB2	1:456:A:GLU:H	4	0.2	0.08	0.2
(1,3152)	1:431:A:TYR:HB3	1:456:A:GLU:H	4	0.2	0.08	0.2
(1,2141)	1:365:A:LYS:HA	1:368:A:ALA:HA	4	0.19	0.03	0.2
(1,1644)	1:325:A:ILE:HD11	1:327:A:SER:H	4	0.19	0.06	0.17
(1,1644)	1:325:A:ILE:HD12	1:327:A:SER:H	4	0.19	0.06	0.17
(1,1644)	1:325:A:ILE:HD13	1:327:A:SER:H	4	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2714)	1:402:A:PHE:HA	1:412:A:GLN:HA	4	0.19	0.04	0.19
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	4	0.19	0.05	0.2
(1,3181)	1:433:A:ILE:H	1:460:A:LEU:H	4	0.18	0.05	0.16
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG2	4	0.18	0.04	0.19
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG3	4	0.18	0.04	0.19
(1,2697)	1:402:A:PHE:HD1	1:461:A:SER:H	4	0.18	0.1	0.12
(1,2697)	1:402:A:PHE:HD2	1:461:A:SER:H	4	0.18	0.1	0.12
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	4	0.16	0.04	0.15
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	4	0.16	0.04	0.15
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	4	0.16	0.04	0.15
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	4	0.16	0.04	0.15
(1,2294)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	4	0.15	0.05	0.16
(1,1254)	1:300:A:TYR:HA	1:306:A:ILE:HB	4	0.15	0.05	0.12
(1,3521)	1:467:A:TRP:HA	1:469:A:MET:H	4	0.14	0.02	0.14
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	4	0.13	0.02	0.13
(1,1196)	1:299:A:LEU:HA	1:325:A:ILE:H	4	0.13	0.01	0.14
(1,1852)	1:345:A:THR:HB	1:346:A:ARG:H	4	0.13	0.03	0.12
(1,2700)	1:402:A:PHE:HD2	1:458:A:LEU:HD13	3	1.24	0.2	1.14
(1,2700)	1:402:A:PHE:HD2	1:458:A:LEU:HD11	3	1.24	0.2	1.14
(1,2700)	1:402:A:PHE:HD1	1:458:A:LEU:HD11	3	1.24	0.2	1.14
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD23	3	0.54	0.16	0.48
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD23	3	0.54	0.16	0.48
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD22	3	0.54	0.16	0.48
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB2	3	0.41	0.07	0.37
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB3	3	0.41	0.07	0.37
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB2	3	0.41	0.07	0.37
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB3	3	0.41	0.07	0.37
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB2	3	0.41	0.07	0.37
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB3	3	0.41	0.07	0.37
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	3	0.4	0.09	0.36
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	3	0.4	0.09	0.36
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	3	0.4	0.09	0.36
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	3	0.4	0.09	0.36
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	3	0.4	0.09	0.36
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	3	0.4	0.09	0.36
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	3	0.36	0.07	0.39
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	3	0.36	0.07	0.39
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE21	3	0.36	0.12	0.44
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE22	3	0.36	0.12	0.44
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	3	0.35	0.03	0.34
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	3	0.35	0.03	0.34
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	3	0.35	0.03	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG2	3	0.35	0.21	0.34
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG3	3	0.35	0.21	0.34
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	3	0.35	0.08	0.34
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	3	0.35	0.08	0.34
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	3	0.35	0.08	0.34
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	3	0.35	0.08	0.34
(1,3383)	1:450:A:LEU:HB2	1:456:A:GLU:H	3	0.35	0.09	0.39
(1,3383)	1:450:A:LEU:HB3	1:456:A:GLU:H	3	0.35	0.09	0.39
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	3	0.34	0.03	0.35
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	3	0.34	0.03	0.35
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD11	3	0.34	0.04	0.31
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD12	3	0.34	0.04	0.31
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD13	3	0.34	0.04	0.31
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD11	3	0.32	0.05	0.35
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD12	3	0.32	0.05	0.35
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD13	3	0.32	0.05	0.35
(1,1829)	1:344:A:VAL:HB	1:348:A:LEU:H	3	0.32	0.02	0.32
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD21	3	0.32	0.06	0.3
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD22	3	0.32	0.06	0.3
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD23	3	0.32	0.06	0.3
(1,1470)	1:314:A:MET:HA	1:353:A:THR:H	3	0.31	0.02	0.32
(1,1780)	1:339:A:LEU:HA	1:345:A:THR:H	3	0.31	0.12	0.34
(1,1021)	1:289:A:TRP:HH2	1:381:A:VAL:H	3	0.31	0.04	0.31
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	3	0.3	0.02	0.3
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	3	0.3	0.02	0.3
(1,1429)	1:312:A:GLN:HE21	1:336:A:ARG:HA	3	0.29	0.09	0.34
(1,1429)	1:312:A:GLN:HE22	1:336:A:ARG:HA	3	0.29	0.09	0.34
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE1	3	0.29	0.09	0.28
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE2	3	0.29	0.09	0.28
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE3	3	0.29	0.09	0.28
(1,2584)	1:394:A:GLU:HA	1:475:A:PHE:HA	3	0.29	0.02	0.28
(1,1333)	1:303:A:ARG:H	1:327:A:SER:H	3	0.29	0.13	0.36
(1,3348)	1:447:A:LEU:HA	1:451:A:ARG:H	3	0.28	0.06	0.25
(1,266)	1:247:A:LYS:HE2	1:263:A:TRP:HH2	3	0.27	0.09	0.31
(1,266)	1:247:A:LYS:HE3	1:263:A:TRP:HH2	3	0.27	0.09	0.31
(1,2478)	1:386:A:PRO:HB2	1:472:A:LEU:HA	3	0.27	0.0	0.27
(1,2478)	1:386:A:PRO:HB3	1:472:A:LEU:HA	3	0.27	0.0	0.27
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	3	0.27	0.04	0.25
(1,1096)	1:296:A:GLY:H	1:309:A:ASP:HA	3	0.27	0.05	0.3
(1,1487)	1:314:A:MET:HG2	1:319:A:ARG:HA	3	0.27	0.06	0.28
(1,1487)	1:314:A:MET:HG3	1:319:A:ARG:HA	3	0.27	0.06	0.28
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	3	0.27	0.14	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	3	0.27	0.14	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	3	0.27	0.14	0.22
(1,672)	1:270:A:GLY:H	1:273:A:GLU:H	3	0.26	0.04	0.24
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	3	0.26	0.06	0.26
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	3	0.26	0.06	0.26
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB2	3	0.25	0.03	0.24
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB3	3	0.25	0.03	0.24
(1,3577)	1:473:A:THR:HA	1:479:A:PRO:HA	3	0.25	0.07	0.21
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG2	3	0.25	0.07	0.23
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG3	3	0.25	0.07	0.23
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG2	3	0.25	0.07	0.23
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG3	3	0.25	0.07	0.23
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD2	3	0.24	0.11	0.17
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD3	3	0.24	0.11	0.17
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB2	3	0.24	0.09	0.3
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB3	3	0.24	0.09	0.3
(1,1129)	1:297:A:LEU:H	1:311:A:GLU:HA	3	0.24	0.04	0.23
(1,1297)	1:301:A:VAL:H	1:306:A:ILE:HB	3	0.24	0.02	0.23
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	3	0.24	0.11	0.23
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	3	0.24	0.11	0.23
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	3	0.24	0.11	0.23
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	3	0.24	0.11	0.23
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD21	3	0.23	0.06	0.25
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD22	3	0.23	0.06	0.25
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD21	3	0.23	0.06	0.25
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD22	3	0.23	0.06	0.25
(1,1503)	1:315:A:PRO:HD2	1:350:A:ASN:HA	3	0.23	0.09	0.26
(1,1503)	1:315:A:PRO:HD3	1:350:A:ASN:HA	3	0.23	0.09	0.26
(1,1541)	1:317:A:TYR:HA	1:320:A:PHE:HD1	3	0.23	0.07	0.25
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	3	0.22	0.07	0.23
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	3	0.22	0.07	0.23
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB2	3	0.22	0.03	0.21
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB3	3	0.22	0.03	0.21
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB2	3	0.22	0.03	0.21
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB3	3	0.22	0.03	0.21
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG2	3	0.22	0.09	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG3	3	0.22	0.09	0.24
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG2	3	0.22	0.09	0.24
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG3	3	0.22	0.09	0.24
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG2	3	0.22	0.09	0.24
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG3	3	0.22	0.09	0.24
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	3	0.22	0.16	0.12
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	3	0.22	0.06	0.2
(1,3570)	1:472:A:LEU:HD21	1:474:A:GLU:HA	3	0.22	0.09	0.26
(1,3570)	1:472:A:LEU:HD22	1:474:A:GLU:HA	3	0.22	0.09	0.26
(1,3570)	1:472:A:LEU:HD23	1:474:A:GLU:HA	3	0.22	0.09	0.26
(1,936)	1:284:A:ALA:HA	1:378:A:PHE:HZ	3	0.22	0.04	0.22
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	3	0.21	0.1	0.2
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	3	0.21	0.1	0.2
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	3	0.21	0.1	0.2
(1,1797)	1:340:A:GLN:HA	1:342:A:SER:H	3	0.21	0.05	0.18
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	3	0.21	0.06	0.21
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	3	0.21	0.09	0.22
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	3	0.21	0.09	0.22
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	3	0.21	0.09	0.22
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	3	0.21	0.09	0.22
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	3	0.21	0.09	0.22
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	3	0.21	0.09	0.22
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	3	0.21	0.07	0.21
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	3	0.21	0.07	0.21
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	3	0.21	0.07	0.21
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	3	0.21	0.07	0.21
(1,3222)	1:436:A:ASP:H	1:441:A:ALA:H	3	0.21	0.02	0.22
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	3	0.21	0.06	0.18
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	3	0.21	0.06	0.18
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	3	0.21	0.07	0.19
(1,575)	1:264:A:SER:HB2	1:356:A:VAL:HA	3	0.21	0.04	0.21
(1,575)	1:264:A:SER:HB3	1:356:A:VAL:HA	3	0.21	0.04	0.21
(1,1348)	1:305:A:PHE:HZ	1:308:A:ASP:HA	3	0.2	0.06	0.24
(1,2009)	1:358:A:GLN:HA	1:361:A:GLU:H	3	0.2	0.05	0.21
(1,3317)	1:444:A:SER:H	1:447:A:LEU:H	3	0.2	0.08	0.2
(1,1352)	1:305:A:PHE:HE1	1:307:A:MET:HA	3	0.2	0.05	0.23
(1,1352)	1:305:A:PHE:HE2	1:307:A:MET:HA	3	0.2	0.05	0.23
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	3	0.19	0.04	0.19
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	3	0.19	0.04	0.19
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	3	0.19	0.07	0.21
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	3	0.19	0.07	0.21
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	3	0.19	0.07	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	3	0.19	0.07	0.21
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	3	0.19	0.07	0.21
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	3	0.19	0.07	0.21
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	3	0.18	0.06	0.14
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	3	0.18	0.06	0.14
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	3	0.18	0.06	0.14
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	3	0.17	0.0	0.17
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	3	0.17	0.0	0.17
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	3	0.17	0.05	0.16
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	3	0.17	0.05	0.16
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	3	0.17	0.05	0.16
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	3	0.17	0.05	0.16
(1,1214)	1:299:A:LEU:H	1:307:A:MET:H	3	0.17	0.03	0.16
(1,3143)	1:431:A:TYR:H	1:458:A:LEU:H	3	0.17	0.05	0.13
(1,1089)	1:296:A:GLY:H	1:311:A:GLU:HA	3	0.16	0.04	0.16
(1,3069)	1:427:A:GLN:HE21	1:455:A:ILE:HA	3	0.16	0.07	0.12
(1,3069)	1:427:A:GLN:HE22	1:455:A:ILE:HA	3	0.16	0.07	0.12
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE21	3	0.15	0.02	0.15
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE22	3	0.15	0.02	0.15
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	3	0.15	0.03	0.16
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	3	0.15	0.03	0.16
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	3	0.14	0.0	0.14
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	3	0.14	0.0	0.14
(1,2680)	1:401:A:ARG:HD2	1:414:A:VAL:H	3	0.13	0.0	0.13
(1,2680)	1:401:A:ARG:HD3	1:414:A:VAL:H	3	0.13	0.0	0.13
(1,3142)	1:431:A:TYR:HA	1:480:A:PHE:HA	3	0.13	0.02	0.14
(1,3464)	1:462:A:ASP:H	1:465:A:ASP:H	3	0.12	0.02	0.12
(1,1381)	1:307:A:MET:HB2	1:308:A:ASP:H	3	0.12	0.01	0.11
(1,1381)	1:307:A:MET:HB3	1:308:A:ASP:H	3	0.12	0.01	0.11
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	2	0.42	0.05	0.42
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	2	0.42	0.05	0.42
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	2	0.38	0.05	0.38
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	2	0.38	0.05	0.38
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD2	2	0.37	0.03	0.37
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD3	2	0.37	0.03	0.37
(1,2569)	1:393:A:GLN:HE21	1:471:A:TYR:HA	2	0.37	0.14	0.37
(1,2569)	1:393:A:GLN:HE22	1:471:A:TYR:HA	2	0.37	0.14	0.37
(1,2367)	1:380:A:LEU:HD22	1:464:A:ILE:H	2	0.36	0.01	0.36
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	2	0.36	0.09	0.36
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	2	0.36	0.09	0.36
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	2	0.35	0.12	0.35
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	2	0.35	0.12	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	2	0.35	0.12	0.35
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD2	2	0.35	0.01	0.35
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD3	2	0.35	0.01	0.35
(1,2572)	1:393:A:GLN:HG2	1:397:A:ALA:H	2	0.34	0.12	0.34
(1,2572)	1:393:A:GLN:HG3	1:397:A:ALA:H	2	0.34	0.12	0.34
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	2	0.33	0.01	0.33
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	2	0.33	0.01	0.33
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	2	0.33	0.01	0.33
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE21	2	0.33	0.03	0.33
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE22	2	0.33	0.03	0.33
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE21	2	0.33	0.03	0.33
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE22	2	0.33	0.03	0.33
(1,1880)	1:348:A:LEU:HD11	1:352:A:LEU:H	2	0.32	0.12	0.32
(1,1880)	1:348:A:LEU:HD12	1:352:A:LEU:H	2	0.32	0.12	0.32
(1,1880)	1:348:A:LEU:HD13	1:352:A:LEU:H	2	0.32	0.12	0.32
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB1	2	0.31	0.04	0.31
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB2	2	0.31	0.04	0.31
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB3	2	0.31	0.04	0.31
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB1	2	0.31	0.04	0.31
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB2	2	0.31	0.04	0.31
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB3	2	0.31	0.04	0.31
(1,2681)	1:401:A:ARG:HD2	1:414:A:VAL:HA	2	0.3	0.08	0.3
(1,2681)	1:401:A:ARG:HD3	1:414:A:VAL:HA	2	0.3	0.08	0.3
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	2	0.3	0.06	0.3
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	2	0.3	0.06	0.3
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	2	0.3	0.06	0.3
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	2	0.3	0.06	0.3
(1,3106)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	2	0.3	0.11	0.3
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD11	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD12	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD13	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD11	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD12	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD13	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD11	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD12	2	0.3	0.01	0.3
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD13	2	0.3	0.01	0.3
(1,268)	1:247:A:LYS:HE2	1:263:A:TRP:HZ3	2	0.29	0.11	0.29
(1,268)	1:247:A:LYS:HE3	1:263:A:TRP:HZ3	2	0.29	0.11	0.29
(1,135)	1:237:A:ASN:HD21	1:240:A:GLU:H	2	0.29	0.04	0.29
(1,135)	1:237:A:ASN:HD22	1:240:A:GLU:H	2	0.29	0.04	0.29
(1,1095)	1:296:A:GLY:HA2	1:309:A:ASP:H	2	0.29	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1095)	1:296:A:GLY:HA3	1:309:A:ASP:H	2	0.29	0.08	0.29
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:HB	2	0.29	0.0	0.29
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE21	2	0.28	0.06	0.28
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE22	2	0.28	0.06	0.28
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	2	0.28	0.03	0.28
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	2	0.28	0.03	0.28
(1,1155)	1:298:A:LYS:H	1:323:A:GLY:H	2	0.28	0.06	0.28
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB2	2	0.28	0.02	0.28
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB3	2	0.28	0.02	0.28
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB2	2	0.28	0.02	0.28
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB3	2	0.28	0.02	0.28
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	2	0.27	0.03	0.27
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	2	0.27	0.03	0.27
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB2	2	0.26	0.06	0.26
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB3	2	0.26	0.06	0.26
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG21	2	0.26	0.12	0.26
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG22	2	0.26	0.12	0.26
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG23	2	0.26	0.12	0.26
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD21	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD22	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD23	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD21	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD22	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD23	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD21	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD22	2	0.26	0.01	0.26
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD23	2	0.26	0.01	0.26
(1,3363)	1:448:A:GLU:HA	1:451:A:ARG:H	2	0.26	0.01	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG21	2	0.26	0.0	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG22	2	0.26	0.0	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG23	2	0.26	0.0	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG21	2	0.26	0.0	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG22	2	0.26	0.0	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG23	2	0.26	0.0	0.26
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB2	2	0.26	0.03	0.26
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB3	2	0.26	0.03	0.26
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB2	2	0.26	0.03	0.26
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB3	2	0.26	0.03	0.26
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB2	2	0.26	0.03	0.26
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB3	2	0.26	0.03	0.26
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB2	2	0.26	0.02	0.26
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB3	2	0.26	0.02	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	2	0.25	0.07	0.25
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	2	0.25	0.03	0.25
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	2	0.25	0.03	0.25
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB2	2	0.25	0.01	0.25
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB3	2	0.25	0.01	0.25
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB2	2	0.25	0.01	0.25
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB3	2	0.25	0.01	0.25
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB2	2	0.25	0.01	0.25
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB3	2	0.25	0.01	0.25
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD11	2	0.25	0.13	0.25
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD12	2	0.25	0.13	0.25
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD13	2	0.25	0.13	0.25
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD2	2	0.24	0.03	0.24
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD3	2	0.24	0.03	0.24
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD2	2	0.24	0.03	0.24
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD3	2	0.24	0.03	0.24
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB2	2	0.24	0.06	0.24
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB3	2	0.24	0.06	0.24
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB2	2	0.24	0.06	0.24
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB3	2	0.24	0.06	0.24
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD11	2	0.24	0.07	0.24
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD12	2	0.24	0.07	0.24
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD13	2	0.24	0.07	0.24
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD11	2	0.24	0.07	0.24
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD12	2	0.24	0.07	0.24
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD13	2	0.24	0.07	0.24
(1,2366)	1:380:A:LEU:HB2	1:464:A:ILE:H	2	0.24	0.05	0.24
(1,2366)	1:380:A:LEU:HB3	1:464:A:ILE:H	2	0.24	0.05	0.24
(1,2758)	1:404:A:SER:HB2	1:458:A:LEU:HA	2	0.24	0.05	0.24
(1,2758)	1:404:A:SER:HB3	1:458:A:LEU:HA	2	0.24	0.05	0.24
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG2	2	0.24	0.08	0.24
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG3	2	0.24	0.08	0.24
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD11	2	0.23	0.02	0.23
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD12	2	0.23	0.02	0.23
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD13	2	0.23	0.02	0.23
(1,3031)	1:423:A:MET:HE1	1:428:A:GLU:HA	2	0.23	0.01	0.23
(1,3031)	1:423:A:MET:HE2	1:428:A:GLU:HA	2	0.23	0.01	0.23
(1,3031)	1:423:A:MET:HE3	1:428:A:GLU:HA	2	0.23	0.01	0.23
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB2	2	0.23	0.06	0.23
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB3	2	0.23	0.06	0.23
(1,339)	1:250:A:TYR:HE1	1:280:A:ILE:HA	2	0.22	0.1	0.22
(1,339)	1:250:A:TYR:HE2	1:280:A:ILE:HA	2	0.22	0.1	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3528)	1:468:A:MET:HA	1:471:A:TYR:H	2	0.22	0.05	0.22
(1,1828)	1:344:A:VAL:HA	1:348:A:LEU:H	2	0.22	0.04	0.22
(1,2387)	1:381:A:VAL:HA	1:385:A:GLY:H	2	0.22	0.04	0.22
(1,1451)	1:313:A:PHE:HZ	1:345:A:THR:HA	2	0.22	0.1	0.22
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD2	2	0.22	0.02	0.22
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD3	2	0.22	0.02	0.22
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB2	2	0.21	0.01	0.21
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB3	2	0.21	0.01	0.21
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	2	0.21	0.05	0.21
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	2	0.21	0.05	0.21
(1,2565)	1:393:A:GLN:HE21	1:473:A:THR:H	2	0.21	0.01	0.21
(1,2565)	1:393:A:GLN:HE22	1:473:A:THR:H	2	0.21	0.01	0.21
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE1	2	0.21	0.09	0.21
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE2	2	0.21	0.09	0.21
(1,2144)	1:365:A:LYS:HA	1:367:A:ASP:H	2	0.2	0.06	0.2
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD11	2	0.2	0.03	0.2
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD12	2	0.2	0.03	0.2
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD13	2	0.2	0.03	0.2
(1,2725)	1:403:A:ALA:H	1:459:A:LEU:H	2	0.2	0.02	0.2
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG21	2	0.2	0.03	0.2
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG22	2	0.2	0.03	0.2
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG23	2	0.2	0.03	0.2
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG21	2	0.2	0.03	0.2
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG22	2	0.2	0.03	0.2
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG23	2	0.2	0.03	0.2
(1,2945)	1:417:A:GLU:HB2	1:418:A:ASP:H	2	0.2	0.0	0.2
(1,2945)	1:417:A:GLU:HB3	1:418:A:ASP:H	2	0.2	0.0	0.2
(1,3263)	1:439:A:ALA:HA	1:442:A:LYS:H	2	0.2	0.03	0.2
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB2	2	0.2	0.09	0.2
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB3	2	0.2	0.09	0.2
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	2	0.2	0.06	0.2
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	2	0.2	0.06	0.2
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	2	0.2	0.06	0.2
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	2	0.2	0.06	0.2
(1,3041)	1:424:A:LYS:H	1:455:A:ILE:HA	2	0.2	0.02	0.2
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	2	0.2	0.01	0.2
(1,666)	1:269:A:GLU:H	1:273:A:GLU:HA	2	0.2	0.02	0.2
(1,1121)	1:297:A:LEU:HD11	1:314:A:MET:HA	2	0.2	0.04	0.2
(1,1121)	1:297:A:LEU:HD12	1:314:A:MET:HA	2	0.2	0.04	0.2
(1,1121)	1:297:A:LEU:HD13	1:314:A:MET:HA	2	0.2	0.04	0.2
(1,3101)	1:429:A:LYS:HA	1:478:A:LYS:HA	2	0.2	0.05	0.2
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD2	2	0.19	0.09	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD3	2	0.19	0.09	0.19
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD2	2	0.19	0.09	0.19
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD3	2	0.19	0.09	0.19
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	2	0.19	0.04	0.19
(1,2374)	1:380:A:LEU:HA	1:384:A:GLU:H	2	0.19	0.07	0.19
(1,3276)	1:440:A:ALA:HA	1:442:A:LYS:H	2	0.19	0.07	0.19
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	2	0.18	0.04	0.18
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	2	0.18	0.04	0.18
(1,2357)	1:379:A:GLY:H	1:382:A:LEU:H	2	0.18	0.02	0.18
(1,2529)	1:388:A:GLU:H	1:390:A:PHE:H	2	0.18	0.06	0.18
(1,1052)	1:293:A:HIS:HB2	1:295:A:HIS:H	2	0.18	0.06	0.18
(1,1052)	1:293:A:HIS:HB3	1:295:A:HIS:H	2	0.18	0.06	0.18
(1,2563)	1:393:A:GLN:HE21	1:474:A:GLU:H	2	0.18	0.05	0.18
(1,2563)	1:393:A:GLN:HE22	1:474:A:GLU:H	2	0.18	0.05	0.18
(1,2828)	1:407:A:THR:HB	1:409:A:SER:H	2	0.18	0.04	0.18
(1,3111)	1:430:A:ILE:H	1:481:A:GLN:H	2	0.18	0.07	0.18
(1,3139)	1:431:A:TYR:HA	1:481:A:GLN:H	2	0.18	0.06	0.18
(1,1351)	1:305:A:PHE:HZ	1:307:A:MET:HA	2	0.18	0.04	0.18
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD2	2	0.18	0.06	0.18
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD3	2	0.18	0.06	0.18
(1,2518)	1:387:A:ALA:HB1	1:467:A:TRP:HH2	2	0.18	0.08	0.18
(1,2518)	1:387:A:ALA:HB2	1:467:A:TRP:HH2	2	0.18	0.08	0.18
(1,2518)	1:387:A:ALA:HB3	1:467:A:TRP:HH2	2	0.18	0.08	0.18
(1,149)	1:238:A:LYS:HA	1:265:A:HIS:HE1	2	0.17	0.03	0.17
(1,418)	1:253:A:ILE:HD11	1:255:A:HIS:H	2	0.17	0.03	0.17
(1,418)	1:253:A:ILE:HD12	1:255:A:HIS:H	2	0.17	0.03	0.17
(1,418)	1:253:A:ILE:HD13	1:255:A:HIS:H	2	0.17	0.03	0.17
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	2	0.17	0.05	0.17
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	2	0.17	0.05	0.17
(1,370)	1:251:A:LYS:HE2	1:259:A:ASP:H	2	0.17	0.04	0.17
(1,370)	1:251:A:LYS:HE3	1:259:A:ASP:H	2	0.17	0.04	0.17
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB2	2	0.17	0.04	0.17
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB3	2	0.17	0.04	0.17
(1,2969)	1:419:A:TYR:HE1	1:431:A:TYR:H	2	0.17	0.01	0.17
(1,2969)	1:419:A:TYR:HE2	1:431:A:TYR:H	2	0.17	0.01	0.17
(1,3578)	1:473:A:THR:HB	1:479:A:PRO:HA	2	0.17	0.02	0.17
(1,1758)	1:337:A:GLU:HA	1:341:A:ASP:H	2	0.16	0.02	0.16
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD11	2	0.16	0.02	0.16
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD12	2	0.16	0.02	0.16
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD13	2	0.16	0.02	0.16
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE2	2	0.16	0.02	0.16
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE3	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,781)	1:277:A:LEU:H	1:324:A:LEU:H	2	0.16	0.03	0.16
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	2	0.16	0.02	0.16
(1,652)	1:268:A:VAL:H	1:273:A:GLU:HA	2	0.16	0.05	0.16
(1,1794)	1:340:A:GLN:HA	1:345:A:THR:HB	2	0.16	0.01	0.16
(1,3505)	1:465:A:ASP:HB2	1:466:A:GLU:H	2	0.16	0.05	0.16
(1,3505)	1:465:A:ASP:HB3	1:466:A:GLU:H	2	0.16	0.05	0.16
(1,269)	1:247:A:LYS:HG2	1:263:A:TRP:HZ3	2	0.15	0.01	0.15
(1,269)	1:247:A:LYS:HG3	1:263:A:TRP:HZ3	2	0.15	0.01	0.15
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	2	0.15	0.02	0.15
(1,1786)	1:339:A:LEU:HA	1:342:A:SER:H	2	0.15	0.02	0.15
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD11	2	0.15	0.01	0.15
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD12	2	0.15	0.01	0.15
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD13	2	0.15	0.01	0.15
(1,3481)	1:464:A:ILE:HA	1:468:A:MET:H	2	0.15	0.02	0.15
(1,1171)	1:298:A:LYS:HA	1:307:A:MET:H	2	0.15	0.03	0.15
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD11	2	0.15	0.02	0.15
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD12	2	0.15	0.02	0.15
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD13	2	0.15	0.02	0.15
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	2	0.14	0.03	0.14
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	2	0.14	0.03	0.14
(1,1762)	1:337:A:GLU:HA	1:340:A:GLN:H	2	0.14	0.03	0.14
(1,467)	1:259:A:ASP:HB2	1:261:A:LEU:HA	2	0.14	0.0	0.14
(1,467)	1:259:A:ASP:HB3	1:261:A:LEU:HA	2	0.14	0.0	0.14
(1,1554)	1:318:A:LEU:HD21	1:374:A:PHE:HZ	2	0.14	0.01	0.14
(1,1554)	1:318:A:LEU:HD22	1:374:A:PHE:HZ	2	0.14	0.01	0.14
(1,1554)	1:318:A:LEU:HD23	1:374:A:PHE:HZ	2	0.14	0.01	0.14
(1,1952)	1:354:A:LYS:HB2	1:358:A:GLN:H	2	0.14	0.0	0.14
(1,1952)	1:354:A:LYS:HB3	1:358:A:GLN:H	2	0.14	0.0	0.14
(1,2683)	1:401:A:ARG:HD2	1:413:A:THR:HA	2	0.14	0.02	0.14
(1,2683)	1:401:A:ARG:HD3	1:413:A:THR:HA	2	0.14	0.02	0.14
(1,3615)	1:475:A:PHE:HD2	1:476:A:ASP:HB3	2	0.14	0.02	0.14
(1,3615)	1:475:A:PHE:HD1	1:476:A:ASP:HB2	2	0.14	0.02	0.14
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA2	2	0.14	0.02	0.14
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA3	2	0.14	0.02	0.14
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA2	2	0.14	0.02	0.14
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA3	2	0.14	0.02	0.14
(1,1090)	1:296:A:GLY:HA2	1:311:A:GLU:HA	2	0.14	0.01	0.14
(1,1090)	1:296:A:GLY:HA3	1:311:A:GLU:HA	2	0.14	0.01	0.14
(1,1139)	1:297:A:LEU:HA	1:309:A:ASP:HA	2	0.14	0.01	0.14
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD21	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD22	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD23	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)
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD21	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD22	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD23	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD21	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD22	2	0.14	0.02	0.14
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD23	2	0.14	0.02	0.14
(1,2939)	1:417:A:GLU:HA	1:420:A:VAL:HB	2	0.14	0.02	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD21	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD22	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD23	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD21	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD22	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD23	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD21	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD22	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD23	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD11	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD12	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD13	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD11	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD12	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD13	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD11	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD12	2	0.14	0.01	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD13	2	0.14	0.01	0.14
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB2	2	0.13	0.03	0.13
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB3	2	0.13	0.03	0.13
(1,2453)	1:384:A:GLU:HA	1:467:A:TRP:HZ3	2	0.13	0.02	0.13
(1,44)	1:233:A:LEU:HD11	1:242:A:THR:H	2	0.12	0.02	0.12
(1,44)	1:233:A:LEU:HD12	1:242:A:THR:H	2	0.12	0.02	0.12
(1,44)	1:233:A:LEU:HD13	1:242:A:THR:H	2	0.12	0.02	0.12
(1,2938)	1:417:A:GLU:HA	1:420:A:VAL:H	2	0.12	0.02	0.12
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG2	2	0.12	0.01	0.12
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG3	2	0.12	0.01	0.12
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG2	2	0.12	0.01	0.12
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG3	2	0.12	0.01	0.12
(1,66)	1:234:A:TRP:HZ2	1:304:A:VAL:H	2	0.12	0.01	0.12
(1,381)	1:251:A:LYS:HA	1:255:A:HIS:H	2	0.12	0.0	0.12
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB2	2	0.12	0.01	0.12
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB3	2	0.12	0.01	0.12
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB2	2	0.12	0.01	0.12
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB3	2	0.12	0.01	0.12

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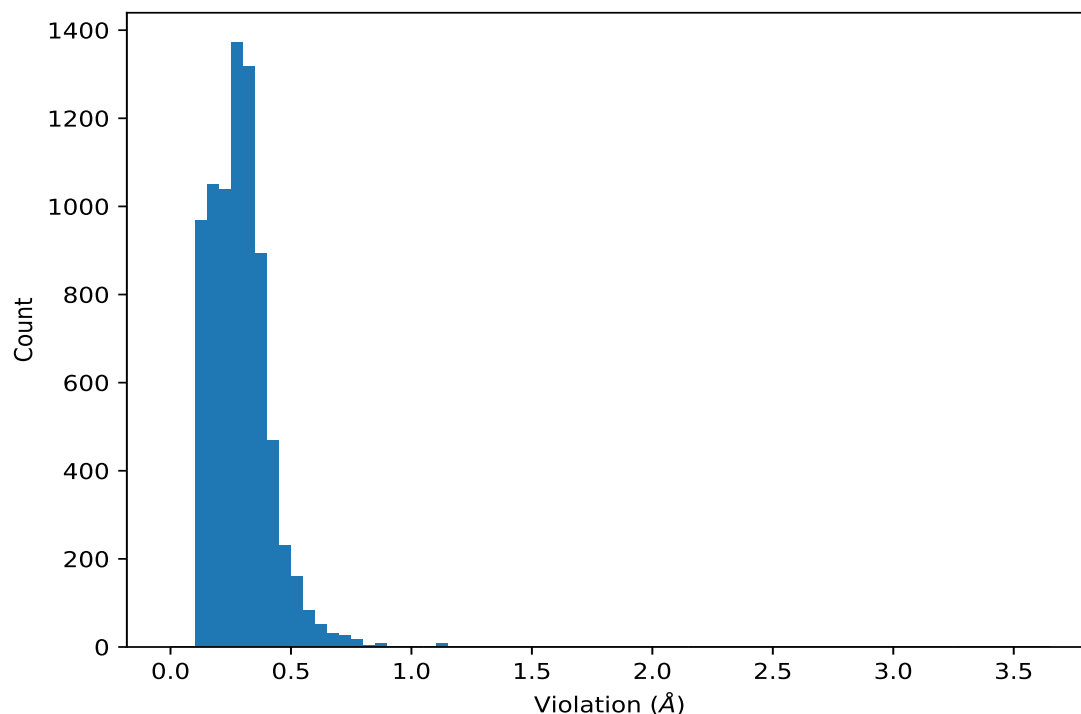
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB2	2	0.12	0.01	0.12
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB3	2	0.12	0.01	0.12
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	2	0.12	0.0	0.12
(1,1317)	1:302:A:GLN:H	1:329:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:234:A:TRP:HZ3	1:249:A:PHE:HZ	2	0.12	0.02	0.12
(1,2935)	1:417:A:GLU:HB2	1:421:A:SER:H	2	0.12	0.02	0.12
(1,2935)	1:417:A:GLU:HB3	1:421:A:SER:H	2	0.12	0.02	0.12
(1,3137)	1:431:A:TYR:HB2	1:482:A:SER:HA	2	0.12	0.0	0.12
(1,3137)	1:431:A:TYR:HB3	1:482:A:SER:HA	2	0.12	0.0	0.12
(1,2734)	1:403:A:ALA:HA	1:414:A:VAL:H	2	0.11	0.01	0.11
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE1	2	0.1	0.0	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE2	2	0.1	0.0	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE3	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)
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	17	3.63
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	13	3.02
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	9	2.71
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	3	2.66
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	12	2.55
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	6	2.4
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	14	2.29
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	4	2.05
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	20	1.69
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	9	1.63
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	7	1.58
(1,2700)	1:402:A:PHE:HD1	1:458:A:LEU:HD11	11	1.52
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	18	1.18
(1,2700)	1:402:A:PHE:HD2	1:458:A:LEU:HD13	19	1.14
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	19	1.13
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	19	1.13
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	19	1.13
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	19	1.13
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	19	1.13
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	19	1.13
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	13	1.11
(1,2700)	1:402:A:PHE:HD2	1:458:A:LEU:HD11	9	1.06
(1,3442)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	18	0.89
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	15	0.88
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	15	0.88
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	15	0.88
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	15	0.88
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	15	0.88
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	15	0.88
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	11	0.88
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	19	0.86
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	15	0.84
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	15	0.84
(1,3442)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	19	0.81
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	5	0.79
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD23	19	0.76
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	10	0.75
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	10	0.75
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	10	0.75
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	10	0.75
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	10	0.75
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE1	2	0.75
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE2	2	0.75
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE3	2	0.75
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE1	2	0.75
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE2	2	0.75
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE3	2	0.75
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE1	2	0.75
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE2	2	0.75
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE3	2	0.75
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	1	0.75
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	14	0.74
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	3	0.72
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	3	0.72
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	3	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	3	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	3	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	3	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	3	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	3	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	3	0.72
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	6	0.71
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	6	0.71
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	6	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	6	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	6	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	6	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	6	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	6	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	6	0.71
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	5	0.7
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	5	0.7
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	5	0.7
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	5	0.7
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	5	0.7
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	5	0.7
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	16	0.69
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	16	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	16	0.69
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	19	0.67
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	19	0.67
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	19	0.67
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	19	0.67
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	3	0.66
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	3	0.66
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	3	0.66
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	3	0.66
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	3	0.66
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	3	0.66
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	11	0.66
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	11	0.66
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	3	0.66
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	6	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	6	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	6	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	6	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	6	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	6	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	13	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	13	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	13	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	13	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	13	0.65
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	13	0.65
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	5	0.65
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	5	0.65
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	12	0.64
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	12	0.64
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	12	0.64
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	12	0.64
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	12	0.64
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	12	0.64
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	2	0.64
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	2	0.64
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD2	15	0.64
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	3	0.63
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	3	0.63
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	3	0.63
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	7	0.63
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	7	0.63
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	7	0.63
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	7	0.63
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	7	0.63
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	2	0.63
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	2	0.63
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	16	0.62
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	16	0.62
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	16	0.62
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	16	0.62
(1,1628)	1:322:A:ARG:HD2	1:323:A:GLY:H	15	0.62
(1,1628)	1:322:A:ARG:HD3	1:323:A:GLY:H	15	0.62
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	14	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	14	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	14	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	14	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	14	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	14	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	17	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	17	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	17	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	17	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	17	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	17	0.61
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	7	0.61
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	7	0.61
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	7	0.61
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG2	15	0.61
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG3	15	0.61
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	6	0.6
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	6	0.6
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	6	0.6
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	14	0.6
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	14	0.6
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	14	0.6
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	14	0.6
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	11	0.59
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	12	0.59
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	12	0.59
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	10	0.59
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	4	0.58
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	4	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	4	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	4	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	4	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	4	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	4	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	4	0.58
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	8	0.58
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	8	0.58
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	8	0.58
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	20	0.58
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	9	0.57
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	9	0.57
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	9	0.57
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	9	0.57
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	9	0.57
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	9	0.57
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	17	0.57
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	17	0.57
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	17	0.57
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	4	0.57
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	4	0.57
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	4	0.57
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	8	0.56
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	8	0.56
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	8	0.56
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	8	0.56
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	1	0.56
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	1	0.56
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	1	0.56
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	1	0.56
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	1	0.56
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	1	0.56
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	12	0.56
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	12	0.56
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	12	0.56
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	12	0.56
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	12	0.56
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	12	0.56
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	12	0.56
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	12	0.56
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	12	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	3	0.56
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	3	0.56
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	7	0.56
(1,3083)	1:428:A:GLU:HG2	1:478:A:LYS:HA	16	0.56
(1,3083)	1:428:A:GLU:HG3	1:478:A:LYS:HA	16	0.56
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	10	0.55
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	10	0.55
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	10	0.55
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	10	0.55
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	10	0.55
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	10	0.55
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	10	0.55
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	10	0.55
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	10	0.55
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	13	0.55
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	13	0.55
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	13	0.55
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	13	0.55
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	13	0.55
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	13	0.55
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	13	0.55
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	13	0.55
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	13	0.55
(1,3442)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	11	0.55
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	11	0.55
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	19	0.55
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	19	0.55
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	20	0.55
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	20	0.55
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	20	0.55
(1,2644)	1:398:A:LYS:HG2	1:417:A:GLU:HG2	4	0.55
(1,2644)	1:398:A:LYS:HG2	1:417:A:GLU:HG3	4	0.55
(1,2644)	1:398:A:LYS:HG3	1:417:A:GLU:HG2	4	0.55
(1,2644)	1:398:A:LYS:HG3	1:417:A:GLU:HG3	4	0.55
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	19	0.54
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	19	0.54
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	19	0.54
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	19	0.54
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	19	0.54
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	19	0.54
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	19	0.54
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	19	0.54
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	4	0.54
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	4	0.54
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	4	0.54
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	4	0.54
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	4	0.54
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	4	0.54
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	19	0.54
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	19	0.54
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	19	0.54
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	19	0.54
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	19	0.54
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	19	0.54
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	19	0.54
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	19	0.54
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	19	0.54
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	3	0.54
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	3	0.54
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	3	0.54
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	3	0.54
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	8	0.53
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	8	0.53
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	8	0.53
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	8	0.53
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	8	0.53
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	8	0.53
(1,2207)	1:371:A:TYR:HD1	1:375:A:TRP:H	7	0.53
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	16	0.53
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	17	0.53
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	9	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	9	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	9	0.52
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	9	0.52
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	9	0.52
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	9	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	9	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	9	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	9	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	11	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	11	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	11	0.52
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	11	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	11	0.52
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	11	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	11	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	11	0.52
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	11	0.52
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	7	0.52
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	7	0.52
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	7	0.52
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	1	0.52
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	1	0.52
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	1	0.52
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	8	0.52
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	12	0.52
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	12	0.52
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	12	0.52
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	1	0.52
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	13	0.52
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	13	0.52
(1,1509)	1:315:A:PRO:HG2	1:319:A:ARG:H	19	0.52
(1,1509)	1:315:A:PRO:HG3	1:319:A:ARG:H	19	0.52
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	7	0.51
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	7	0.51
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	7	0.51
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	7	0.51
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	7	0.51
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	7	0.51
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	7	0.51
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	7	0.51
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	7	0.51
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	16	0.51
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	16	0.51
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	16	0.51
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	16	0.51
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	16	0.51
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	16	0.51
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	16	0.51
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	16	0.51
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	16	0.51
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	2	0.51
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	2	0.51
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	2	0.51
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	18	0.51
(1,2569)	1:393:A:GLN:HE21	1:471:A:TYR:HA	14	0.51
(1,2569)	1:393:A:GLN:HE22	1:471:A:TYR:HA	14	0.51
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	4	0.51
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	4	0.51
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	4	0.51
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	4	0.51
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	7	0.51
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	12	0.5
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	12	0.5
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	12	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	12	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	12	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	12	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	12	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	12	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	12	0.5
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	17	0.5
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	17	0.5
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	17	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	17	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	17	0.5
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	17	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	17	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	17	0.5
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	17	0.5
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	11	0.5
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	11	0.5
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	11	0.5
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	20	0.5
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	20	0.5
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	20	0.5
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	3	0.5
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	3	0.5
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	3	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	3	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	3	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	3	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	3	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	3	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	3	0.5
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	13	0.5
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	13	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	13	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	13	0.5
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	13	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	13	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	13	0.5
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	13	0.5
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB2	1	0.5
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB3	1	0.5
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB2	1	0.5
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB3	1	0.5
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB2	1	0.5
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB3	1	0.5
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	5	0.5
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	5	0.5
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD11	16	0.5
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD12	16	0.5
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD13	16	0.5
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	1	0.5
(1,2024)	1:359:A:MET:HA	1:362:A:LYS:HD2	5	0.5
(1,2024)	1:359:A:MET:HA	1:362:A:LYS:HD3	5	0.5
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	3	0.5
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	3	0.5
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	3	0.5
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	12	0.49
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	12	0.49
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	12	0.49
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	5	0.49
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	5	0.49
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	5	0.49
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	5	0.49
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	5	0.49
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	5	0.49
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	5	0.49
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	5	0.49
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	5	0.49
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	8	0.49
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	8	0.49
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	8	0.49
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	2	0.49
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	2	0.49
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	2	0.49
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	1	0.49
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	4	0.49
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	13	0.48
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	15	0.48
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	15	0.48
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	15	0.48
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	15	0.48
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	15	0.48
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	15	0.48
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	15	0.48
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	15	0.48
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	15	0.48
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	16	0.48
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	16	0.48
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	16	0.48
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	17	0.48
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	17	0.48
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	17	0.48
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	4	0.48
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	18	0.48
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	6	0.48
(1,1509)	1:315:A:PRO:HG2	1:319:A:ARG:H	5	0.48
(1,1509)	1:315:A:PRO:HG3	1:319:A:ARG:H	5	0.48
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	18	0.48
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	3	0.48
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD23	3	0.48
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	15	0.48
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	15	0.48
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	10	0.48
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	20	0.48
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	20	0.48
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	11	0.47
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	11	0.47
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	11	0.47
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	11	0.47
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	11	0.47
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	11	0.47
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	11	0.47
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	11	0.47
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	1	0.47
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	1	0.47
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	1	0.47
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	1	0.47
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	1	0.47
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	1	0.47
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	1	0.47
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	1	0.47
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	1	0.47
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	18	0.47
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	18	0.47
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	18	0.47
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	18	0.47
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	18	0.47
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	18	0.47
(1,3569)	1:472:A:LEU:HD21	1:474:A:GLU:H	10	0.47
(1,3569)	1:472:A:LEU:HD22	1:474:A:GLU:H	10	0.47
(1,3569)	1:472:A:LEU:HD23	1:474:A:GLU:H	10	0.47
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	14	0.47
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	14	0.47
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	6	0.47
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	6	0.47
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	8	0.47
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	8	0.47
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	8	0.47
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	8	0.47
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	4	0.47
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	4	0.47
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	4	0.47
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	11	0.47
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	11	0.47
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	11	0.47
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	14	0.47
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	16	0.47
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	16	0.47
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	19	0.47
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	19	0.47
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	19	0.47
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	19	0.47
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	14	0.46
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	14	0.46
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	14	0.46
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	14	0.46
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	14	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	14	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	14	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	14	0.46
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	12	0.46
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	12	0.46
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	12	0.46
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	12	0.46
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	16	0.46
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	16	0.46
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	16	0.46
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	16	0.46
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	16	0.46
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	16	0.46
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	11	0.46
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	11	0.46
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	11	0.46
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	11	0.46
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	11	0.46
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	11	0.46
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	11	0.46
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	11	0.46
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	11	0.46
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	1	0.46
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	1	0.46
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	1	0.46
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	19	0.46
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	19	0.46
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	19	0.46
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	7	0.46
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	7	0.46
(1,3385)	1:450:A:LEU:HA	1:455:A:ILE:HB	16	0.46
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	12	0.46
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	12	0.46
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	12	0.46
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	7	0.46
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	7	0.46
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	18	0.46
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	18	0.46
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	18	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	11	0.46
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	11	0.46
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	11	0.46
(1,2572)	1:393:A:GLN:HG2	1:397:A:ALA:H	17	0.46
(1,2572)	1:393:A:GLN:HG3	1:397:A:ALA:H	17	0.46
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	1	0.46
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	1	0.46
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	1	0.46
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	1	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	1	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	1	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	1	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	7	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	7	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	7	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	10	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	10	0.46
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	10	0.46
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	3	0.46
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	20	0.46
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	20	0.46
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	20	0.46
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	8	0.46
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	20	0.46
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	20	0.46
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	20	0.46
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	20	0.46
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	5	0.46
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	19	0.46
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	20	0.46
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	15	0.46
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	20	0.45
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	20	0.45
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	20	0.45
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	20	0.45
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	20	0.45
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	20	0.45
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	20	0.45
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	20	0.45
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	20	0.45
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	9	0.45
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	9	0.45
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	9	0.45
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	5	0.45
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	5	0.45
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	5	0.45
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	5	0.45
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	5	0.45
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	5	0.45
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	5	0.45
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	5	0.45
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	5	0.45
(1,3565)	1:472:A:LEU:HD22	1:480:A:PHE:HE1	2	0.45
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB2	2	0.45
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB3	2	0.45
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	1	0.45
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	1	0.45
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	1	0.45
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	8	0.45
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	8	0.45
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	8	0.45
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	15	0.45
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	20	0.45
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	15	0.45
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	15	0.45
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	13	0.45
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	13	0.45
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	13	0.45
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	13	0.45
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	8	0.45
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	8	0.45
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	8	0.45
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	8	0.45
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	10	0.45
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	10	0.45
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	10	0.45
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	10	0.45
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	3	0.45
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	3	0.45
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	3	0.45
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	2	0.45
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	2	0.45
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	1	0.45
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	7	0.45
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	20	0.45
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	7	0.44
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	20	0.44
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	9	0.44
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	9	0.44
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	9	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	11	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	11	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	11	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	14	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	14	0.44
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	14	0.44
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	4	0.44
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	4	0.44
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	4	0.44
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	4	0.44
(1,3383)	1:450:A:LEU:HB2	1:456:A:GLU:H	17	0.44
(1,3383)	1:450:A:LEU:HB3	1:456:A:GLU:H	17	0.44
(1,3200)	1:434:A:THR:HA	1:461:A:SER:HA	20	0.44
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	11	0.44
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	11	0.44
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	11	0.44
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	11	0.44
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	3	0.44
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	3	0.44
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	3	0.44
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	20	0.44
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	20	0.44
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	14	0.44
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	14	0.44
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	14	0.44
(1,2862)	1:410:A:SER:HB3	1:438:A:TYR:HD2	2	0.44
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	6	0.44
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	9	0.44
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE21	1	0.44
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE22	1	0.44
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE21	9	0.44
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE22	9	0.44
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	10	0.44
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	10	0.44
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	12	0.44
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	12	0.44
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	12	0.44
(1,1880)	1:348:A:LEU:HD11	1:352:A:LEU:H	6	0.44
(1,1880)	1:348:A:LEU:HD12	1:352:A:LEU:H	6	0.44
(1,1880)	1:348:A:LEU:HD13	1:352:A:LEU:H	6	0.44
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	17	0.44
(1,1780)	1:339:A:LEU:HA	1:345:A:THR:H	13	0.44
(1,1760)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	2	0.44
(1,1760)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	2	0.44
(1,1760)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	2	0.44
(1,1760)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	2	0.44
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	2	0.44
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	2	0.44
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	2	0.44
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	2	0.44
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	9	0.44
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	9	0.44
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	9	0.44
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	9	0.44
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	18	0.44
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	18	0.44
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	19	0.44
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	19	0.44
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	5	0.44
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	9	0.44
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	15	0.44
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	9	0.44
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	9	0.44
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	18	0.44
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	3	0.43
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	10	0.43
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	10	0.43
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	10	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	17	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	17	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	17	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	19	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	19	0.43
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	19	0.43
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	16	0.43
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	16	0.43
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	16	0.43
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	16	0.43
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	16	0.43
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	16	0.43
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	16	0.43
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	16	0.43
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB2	19	0.43
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB3	19	0.43
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	19	0.43
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	19	0.43
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	18	0.43
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	18	0.43
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	18	0.43
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	18	0.43
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	19	0.43
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	19	0.43
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	19	0.43
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	19	0.43
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	13	0.43
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	13	0.43
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	13	0.43
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	16	0.43
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	16	0.43
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	16	0.43
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	16	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	9	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	9	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	9	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	12	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	12	0.43
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	12	0.43
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	10	0.43
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	10	0.43
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	10	0.43
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	10	0.43
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	10	0.43
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	10	0.43
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	20	0.43
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	20	0.43
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	6	0.43
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	6	0.43
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	6	0.43
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	6	0.43
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	6	0.43
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	6	0.43
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	2	0.43
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	6	0.43
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	15	0.43
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	14	0.43
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	14	0.43
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	5	0.43
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	6	0.43
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	17	0.43
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	13	0.43
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	14	0.43
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	7	0.42
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	7	0.42
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	7	0.42
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	7	0.42
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	17	0.42
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	17	0.42
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	17	0.42
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	17	0.42
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	2	0.42
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	2	0.42
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	2	0.42
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	2	0.42
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	2	0.42
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	2	0.42
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	5	0.42
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	5	0.42
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	5	0.42
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	5	0.42
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	5	0.42
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	5	0.42
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	5	0.42
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	5	0.42
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	5	0.42
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	20	0.42
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	20	0.42
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	20	0.42
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	20	0.42
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	20	0.42
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	12	0.42
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	12	0.42
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	12	0.42
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	12	0.42
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	12	0.42
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	12	0.42
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	12	0.42
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	12	0.42
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	12	0.42
(1,3660)	1:447:A:LEU:HD21	2:607:B:ILE:HD11	12	0.42
(1,3660)	1:447:A:LEU:HD21	2:607:B:ILE:HD12	12	0.42
(1,3660)	1:447:A:LEU:HD21	2:607:B:ILE:HD13	12	0.42
(1,3660)	1:447:A:LEU:HD22	2:607:B:ILE:HD11	12	0.42
(1,3660)	1:447:A:LEU:HD22	2:607:B:ILE:HD12	12	0.42
(1,3660)	1:447:A:LEU:HD22	2:607:B:ILE:HD13	12	0.42
(1,3660)	1:447:A:LEU:HD23	2:607:B:ILE:HD11	12	0.42
(1,3660)	1:447:A:LEU:HD23	2:607:B:ILE:HD12	12	0.42
(1,3660)	1:447:A:LEU:HD23	2:607:B:ILE:HD13	12	0.42
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	14	0.42
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	14	0.42
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	14	0.42
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	8	0.42
(1,3385)	1:450:A:LEU:HA	1:455:A:ILE:HB	18	0.42
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	12	0.42
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	19	0.42
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	7	0.42
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	7	0.42
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	13	0.42
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	12	0.42
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	12	0.42
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	12	0.42
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	12	0.42
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	16	0.42
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	16	0.42
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	14	0.42
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	14	0.42
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	14	0.42
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	14	0.42
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	7	0.42
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	18	0.42
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	18	0.42
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	18	0.42
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	18	0.42
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	18	0.42
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	18	0.42
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	19	0.42
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	19	0.42
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	19	0.42
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	19	0.42
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	19	0.42
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	19	0.42
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	14	0.42
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	5	0.42
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	7	0.42
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	7	0.42
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	7	0.42
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	8	0.42
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	15	0.42
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	15	0.42
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	15	0.42
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	15	0.42
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	15	0.42
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	15	0.42
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	15	0.42
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	15	0.42
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	15	0.42
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	1	0.42
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	1	0.42
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	1	0.42
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	1	0.42
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	11	0.42
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	11	0.42
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	11	0.42
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	11	0.42
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	15	0.42
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	15	0.42
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	15	0.42
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	15	0.42
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	4	0.42
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	16	0.42
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	16	0.42
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	6	0.42
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	6	0.42
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	1	0.42
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	1	0.42
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	1	0.42
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	11	0.42
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	11	0.42
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	11	0.42
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	14	0.42
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	14	0.42
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	12	0.42
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	8	0.42
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	8	0.42
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	8	0.42
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	8	0.42
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	8	0.42
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	8	0.42
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	7	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	9	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	9	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	9	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	18	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	18	0.41
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	18	0.41
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	13	0.41
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	13	0.41
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	13	0.41
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	13	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	6	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	6	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	6	0.41
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	6	0.41
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	6	0.41
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	6	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	6	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	6	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	6	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	18	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	18	0.41
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	18	0.41
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	18	0.41
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	18	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	18	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	18	0.41
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	18	0.41
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	11	0.41
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	11	0.41
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	11	0.41
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	11	0.41
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	11	0.41
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	11	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	3	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	3	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	3	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	3	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	3	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	3	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	3	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	3	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	3	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	10	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	10	0.41
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	10	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	10	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	10	0.41
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	10	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	10	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	10	0.41
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	10	0.41
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	19	0.41
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	19	0.41
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	19	0.41
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	19	0.41
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	19	0.41
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	19	0.41
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	19	0.41
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	19	0.41
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	19	0.41
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	18	0.41
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	18	0.41
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3375)	1:449:A:LEU:HA	1:452:A:LYS:HB2	15	0.41
(1,3375)	1:449:A:LEU:HA	1:452:A:LYS:HB3	15	0.41
(1,3106)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	20	0.41
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD2	15	0.41
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD3	15	0.41
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	19	0.41
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	19	0.41
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	19	0.41
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	4	0.41
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	6	0.41
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	6	0.41
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	6	0.41
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	2	0.41
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	7	0.41
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	7	0.41
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	7	0.41
(1,1509)	1:315:A:PRO:HG2	1:319:A:ARG:H	16	0.41
(1,1509)	1:315:A:PRO:HG3	1:319:A:ARG:H	16	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	6	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	6	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	6	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	19	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	19	0.41
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	19	0.41
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	7	0.41
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	7	0.41
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	12	0.41
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	12	0.41
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	17	0.41
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	17	0.41
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	17	0.41
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	18	0.41
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	18	0.41
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	18	0.41
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	2	0.41
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	15	0.41
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	14	0.4
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	14	0.4
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	14	0.4
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	14	0.4
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	14	0.4
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	14	0.4
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	14	0.4
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	14	0.4
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	5	0.4
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	5	0.4
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	5	0.4
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	9	0.4
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	9	0.4
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	9	0.4
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	9	0.4
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	9	0.4
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	9	0.4
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	9	0.4
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	9	0.4
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	9	0.4
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	8	0.4
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	8	0.4
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	8	0.4
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	8	0.4
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	8	0.4
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	8	0.4
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	8	0.4
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	8	0.4
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	8	0.4
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	20	0.4
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	20	0.4
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	20	0.4
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	4	0.4
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	18	0.4
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	18	0.4
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	18	0.4
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	9	0.4
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	9	0.4
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	9	0.4
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD21	11	0.4
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD22	11	0.4
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD23	11	0.4
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	20	0.4
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	12	0.4
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	13	0.4
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	15	0.4
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD11	11	0.4
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD12	11	0.4
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD13	11	0.4
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	15	0.4
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	15	0.4
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	15	0.4
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	15	0.4
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	15	0.4
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	15	0.4
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE1	12	0.4
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE2	12	0.4
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE3	12	0.4
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	10	0.4
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	10	0.4
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	10	0.4
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	10	0.4
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	10	0.4
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	10	0.4
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	5	0.4
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	5	0.4
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	5	0.4
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	5	0.4
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	14	0.4
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	14	0.4
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	12	0.4
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	12	0.4
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	4	0.4
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD2	15	0.4
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD3	15	0.4
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	16	0.4
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	16	0.4
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	15	0.4
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	15	0.4
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	15	0.4
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	15	0.4
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	4	0.4
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	1	0.4
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	1	0.4
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	12	0.4
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	12	0.4
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	11	0.4
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	20	0.4
(1,268)	1:247:A:LYS:HE2	1:263:A:TRP:HZ3	14	0.4
(1,268)	1:247:A:LYS:HE3	1:263:A:TRP:HZ3	14	0.4
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	8	0.4
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	8	0.4
(1,109)	1:235:A:THR:HA	1:267:A:ARG:HD2	13	0.4
(1,109)	1:235:A:THR:HA	1:267:A:ARG:HD3	13	0.4
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	19	0.4
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	1	0.4
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	17	0.4
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	16	0.39
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	16	0.39
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	16	0.39
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	16	0.39
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	16	0.39
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	16	0.39
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	16	0.39
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	16	0.39
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	16	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	17	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	17	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	17	0.39
(1,3680)	1:317:A:TYR:HE1	2:626:B:PHE:HD1	16	0.39
(1,3680)	1:317:A:TYR:HE1	2:626:B:PHE:HD2	16	0.39
(1,3680)	1:317:A:TYR:HE2	2:626:B:PHE:HD1	16	0.39
(1,3680)	1:317:A:TYR:HE2	2:626:B:PHE:HD2	16	0.39
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	10	0.39
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	10	0.39
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	10	0.39
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	10	0.39
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	16	0.39
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	16	0.39
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	16	0.39
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	16	0.39
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	5	0.39
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	5	0.39
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	5	0.39
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	5	0.39
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	5	0.39
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	5	0.39
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	5	0.39
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	5	0.39
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	17	0.39
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	17	0.39
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	17	0.39
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	17	0.39
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	17	0.39
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	17	0.39
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	17	0.39
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	17	0.39
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	17	0.39
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	15	0.39
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	15	0.39
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	15	0.39
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	15	0.39
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	15	0.39
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	15	0.39
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	15	0.39
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	15	0.39
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	15	0.39
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	6	0.39
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	6	0.39
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	6	0.39
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	10	0.39
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	10	0.39
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	10	0.39
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB2	2	0.39
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB3	2	0.39
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB2	17	0.39
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB3	17	0.39
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG21	18	0.39
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG22	18	0.39
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG23	18	0.39
(1,3383)	1:450:A:LEU:HB2	1:456:A:GLU:H	6	0.39
(1,3383)	1:450:A:LEU:HB3	1:456:A:GLU:H	6	0.39
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	4	0.39
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	4	0.39
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	18	0.39
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	18	0.39
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	4	0.39
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	15	0.39
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	15	0.39
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	19	0.39
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	13	0.39
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	13	0.39
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	13	0.39
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	13	0.39
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG2	18	0.39
(1,2947)	1:418:A:ASP:HA	1:422:A:ARG:HG3	18	0.39
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	20	0.39
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	20	0.39
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	20	0.39
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	1	0.39
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	1	0.39
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	1	0.39
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	1	0.39
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	1	0.39
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	1	0.39
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	20	0.39
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	5	0.39
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	5	0.39
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	5	0.39
(1,2369)	1:380:A:LEU:HD11	1:463:A:ARG:H	4	0.39
(1,2369)	1:380:A:LEU:HD12	1:463:A:ARG:H	4	0.39
(1,2369)	1:380:A:LEU:HD13	1:463:A:ARG:H	4	0.39
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	7	0.39
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	7	0.39
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	5	0.39
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	5	0.39
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	5	0.39
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	5	0.39
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	5	0.39
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	5	0.39
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	12	0.39
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	12	0.39
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	5	0.39
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	5	0.39
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	5	0.39
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	5	0.39
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	5	0.39
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	5	0.39
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	5	0.39
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	5	0.39
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	13	0.39
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	13	0.39
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	13	0.39
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	13	0.39
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	8	0.39
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	8	0.39
(1,1333)	1:303:A:ARG:H	1:327:A:SER:H	11	0.39
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD2	15	0.39
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD3	15	0.39
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	8	0.39
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	13	0.39
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	9	0.39
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	9	0.39
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	9	0.39
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	10	0.39
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	10	0.39
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	10	0.39
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	20	0.39
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	20	0.39
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	20	0.39
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	20	0.39
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	20	0.39
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	17	0.39
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	3	0.39
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	12	0.39
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	17	0.39
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	9	0.39
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	4	0.39
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	4	0.39
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	4	0.39
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	19	0.39
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	19	0.39
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	19	0.39
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	1	0.38
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	1	0.38
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	1	0.38
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	12	0.38
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	12	0.38
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	12	0.38
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	12	0.38
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	12	0.38
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	12	0.38
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	12	0.38
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	12	0.38
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	4	0.38
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	4	0.38
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	4	0.38
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	15	0.38
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	15	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	15	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	15	0.38
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	9	0.38
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	9	0.38
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	9	0.38
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	9	0.38
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	9	0.38
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	9	0.38
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	3	0.38
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	3	0.38
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	3	0.38
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	3	0.38
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	3	0.38
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	3	0.38
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	3	0.38
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	3	0.38
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	3	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	6	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	6	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	6	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	6	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	6	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	6	0.38
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	6	0.38
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	6	0.38
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	6	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	18	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	18	0.38
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	18	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	18	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	18	0.38
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	18	0.38
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	18	0.38
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	18	0.38
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	18	0.38
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	18	0.38
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	18	0.38
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	18	0.38
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	18	0.38
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	18	0.38
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	18	0.38
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	18	0.38
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	18	0.38
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	11	0.38
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	11	0.38
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	11	0.38
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	1	0.38
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	1	0.38
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	1	0.38
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	2	0.38
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	1	0.38
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	9	0.38
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	9	0.38
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	9	0.38
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	9	0.38
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	4	0.38
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	4	0.38
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	4	0.38
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	11	0.38
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	11	0.38
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	11	0.38
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	11	0.38
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	11	0.38
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	11	0.38
(1,3022)	1:423:A:MET:HA	1:456:A:GLU:H	11	0.38
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	2	0.38
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	2	0.38
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	14	0.38
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	14	0.38
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	14	0.38
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	14	0.38
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	14	0.38
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	14	0.38
(1,2681)	1:401:A:ARG:HD2	1:414:A:VAL:HA	8	0.38
(1,2681)	1:401:A:ARG:HD3	1:414:A:VAL:HA	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	6	0.38
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	6	0.38
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	6	0.38
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	10	0.38
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	10	0.38
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	20	0.38
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	20	0.38
(1,2568)	1:393:A:GLN:HE21	1:472:A:LEU:HD21	10	0.38
(1,2568)	1:393:A:GLN:HE21	1:472:A:LEU:HD22	10	0.38
(1,2568)	1:393:A:GLN:HE21	1:472:A:LEU:HD23	10	0.38
(1,2568)	1:393:A:GLN:HE22	1:472:A:LEU:HD21	10	0.38
(1,2568)	1:393:A:GLN:HE22	1:472:A:LEU:HD22	10	0.38
(1,2568)	1:393:A:GLN:HE22	1:472:A:LEU:HD23	10	0.38
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	10	0.38
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	10	0.38
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	10	0.38
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	10	0.38
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	11	0.38
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	11	0.38
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	11	0.38
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	11	0.38
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD11	8	0.38
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD12	8	0.38
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD13	8	0.38
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	8	0.38
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	6	0.38
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	9	0.38
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	20	0.38
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	20	0.38
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	20	0.38
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	20	0.38
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	20	0.38
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	20	0.38
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	15	0.38
(1,2207)	1:371:A:TYR:HD1	1:375:A:TRP:H	11	0.38
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	6	0.38
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	6	0.38
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	6	0.38
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	6	0.38
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	9	0.38
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	9	0.38
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	8	0.38
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	8	0.38
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	18	0.38
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	20	0.38
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	3	0.38
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	3	0.38
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	3	0.38
(1,1509)	1:315:A:PRO:HG2	1:319:A:ARG:H	3	0.38
(1,1509)	1:315:A:PRO:HG3	1:319:A:ARG:H	3	0.38
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	7	0.38
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	7	0.38
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	7	0.38
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	7	0.38
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	16	0.38
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	16	0.38
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	3	0.38
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	3	0.38
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	18	0.38
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	6	0.38
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	6	0.38
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	6	0.38
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	6	0.38
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	6	0.38
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	6	0.38
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	1	0.38
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	1	0.38
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	19	0.38
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	19	0.38
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	20	0.38
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	20	0.38
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	20	0.38
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	8	0.38
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	8	0.38
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	19	0.38
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	19	0.38
(1,1065)	1:295:A:HIS:HB2	1:320:A:PHE:HA	19	0.38
(1,1065)	1:295:A:HIS:HB3	1:320:A:PHE:HA	19	0.38
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	7	0.38
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	11	0.38
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	20	0.38
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	5	0.38
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	20	0.38
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	2	0.38
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	2	0.38
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	2	0.38
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	9	0.38
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	2	0.38
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	10	0.38
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	1	0.37
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	1	0.37
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	1	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	1	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	1	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	1	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	1	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	1	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	1	0.37
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	4	0.37
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	4	0.37
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	4	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	4	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	4	0.37
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	4	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	4	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	4	0.37
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	4	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	12	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	12	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	12	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	15	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	15	0.37
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	15	0.37
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	19	0.37
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	19	0.37
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	19	0.37
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	19	0.37
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	19	0.37
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	19	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	3	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	3	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	3	0.37
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	3	0.37
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	3	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	3	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	3	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	3	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	13	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	13	0.37
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	13	0.37
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	13	0.37
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	13	0.37
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	13	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	13	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	13	0.37
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	13	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	2	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	2	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	2	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	2	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	2	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	2	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	2	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	2	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	2	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	17	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	17	0.37
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	17	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	17	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	17	0.37
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	17	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	17	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	17	0.37
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	17	0.37
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	6	0.37
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	6	0.37
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	6	0.37
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	6	0.37
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	6	0.37
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	6	0.37
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	6	0.37
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	6	0.37
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	6	0.37
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	7	0.37
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	7	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	7	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	7	0.37
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	7	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	7	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	7	0.37
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	7	0.37
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB2	20	0.37
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB3	20	0.37
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB2	20	0.37
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB3	20	0.37
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB2	20	0.37
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB3	20	0.37
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	2	0.37
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	2	0.37
(1,3499)	1:465:A:ASP:HA	1:468:A:MET:HE1	4	0.37
(1,3499)	1:465:A:ASP:HA	1:468:A:MET:HE2	4	0.37
(1,3499)	1:465:A:ASP:HA	1:468:A:MET:HE3	4	0.37
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	2	0.37
(1,3348)	1:447:A:LEU:HA	1:451:A:ARG:H	10	0.37
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	3	0.37
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	3	0.37
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	9	0.37
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	17	0.37
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	3	0.37
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	3	0.37
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	3	0.37
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	12	0.37
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	12	0.37
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	12	0.37
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	12	0.37
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	12	0.37
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	12	0.37
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	2	0.37
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	2	0.37
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	2	0.37
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	12	0.37
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	18	0.37
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	18	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	18	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	18	0.37
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	19	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	19	0.37
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	19	0.37
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	3	0.37
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	4	0.37
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	9	0.37
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	17	0.37
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD11	15	0.37
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD12	15	0.37
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD13	15	0.37
(1,2469)	1:385:A:GLY:HA2	1:389:A:ASP:H	11	0.37
(1,2469)	1:385:A:GLY:HA3	1:389:A:ASP:H	11	0.37
(1,2367)	1:380:A:LEU:HD22	1:464:A:ILE:H	6	0.37
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	4	0.37
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	4	0.37
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	4	0.37
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	4	0.37
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	5	0.37
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	11	0.37
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	11	0.37
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	1	0.37
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	1	0.37
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	1	0.37
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	1	0.37
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	1	0.37
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	1	0.37
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	1	0.37
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	1	0.37
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	1	0.37
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	14	0.37
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	14	0.37
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	10	0.37
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	10	0.37
(1,1480)	1:314:A:MET:HA	1:349:A:ARG:HG2	13	0.37
(1,1480)	1:314:A:MET:HA	1:349:A:ARG:HG3	13	0.37
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	2	0.37
(1,1429)	1:312:A:GLN:HE21	1:336:A:ARG:HA	6	0.37
(1,1429)	1:312:A:GLN:HE22	1:336:A:ARG:HA	6	0.37
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	16	0.37
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	16	0.37
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	9	0.37
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	3	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	3	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	3	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	11	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	11	0.37
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	11	0.37
(1,1095)	1:296:A:GLY:HA2	1:309:A:ASP:H	2	0.37
(1,1095)	1:296:A:GLY:HA3	1:309:A:ASP:H	2	0.37
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD11	17	0.37
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD12	17	0.37
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD13	17	0.37
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	1	0.37
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	18	0.37
(1,917)	1:282:A:SER:HA	1:374:A:PHE:HA	15	0.37
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD22	12	0.37
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	7	0.37
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	7	0.37
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	7	0.37
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	3	0.37
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	3	0.37
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	17	0.37
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	8	0.37
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	16	0.37
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	19	0.37
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	19	0.37
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	19	0.37
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	19	0.37
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	19	0.37
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	19	0.37
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	13	0.37
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	13	0.37
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	14	0.37
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	16	0.37
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	2	0.37
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	15	0.37
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	12	0.37
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	12	0.37
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	12	0.37
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	12	0.37
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	20	0.37
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	20	0.37
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	5	0.37
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	15	0.37
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	13	0.36
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	13	0.36
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	13	0.36
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	13	0.36
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	13	0.36
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	13	0.36
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	13	0.36
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	13	0.36
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	13	0.36
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	17	0.36
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	17	0.36
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	17	0.36
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	10	0.36
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	10	0.36
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	10	0.36
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	9	0.36
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	9	0.36
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	9	0.36
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	9	0.36
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	9	0.36
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	9	0.36
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	9	0.36
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	9	0.36
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	9	0.36
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	7	0.36
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	7	0.36
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	7	0.36
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	7	0.36
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	7	0.36
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	7	0.36
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	7	0.36
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	7	0.36
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	7	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	7	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	7	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	7	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	7	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	7	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	7	0.36
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	7	0.36
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	7	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	10	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	10	0.36
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	10	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	10	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	10	0.36
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	10	0.36
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	10	0.36
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	10	0.36
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	10	0.36
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	19	0.36
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	19	0.36
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	12	0.36
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	12	0.36
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	12	0.36
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	20	0.36
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	20	0.36
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	20	0.36
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	20	0.36
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	20	0.36
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	20	0.36
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	4	0.36
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	4	0.36
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	4	0.36
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	3	0.36
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	5	0.36
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	13	0.36
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	13	0.36
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	13	0.36
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	2	0.36
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	2	0.36
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	2	0.36
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	2	0.36
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	3	0.36
(1,2957)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	3	0.36
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	16	0.36
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	11	0.36
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	11	0.36
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	11	0.36
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	11	0.36
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	11	0.36
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	5	0.36
(1,2605)	1:395:A:ALA:HA	1:397:A:ALA:H	20	0.36
(1,2585)	1:394:A:GLU:HG2	1:475:A:PHE:HA	6	0.36
(1,2585)	1:394:A:GLU:HG3	1:475:A:PHE:HA	6	0.36
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	14	0.36
(1,2564)	1:393:A:GLN:HE21	1:474:A:GLU:HB2	4	0.36
(1,2564)	1:393:A:GLN:HE21	1:474:A:GLU:HB3	4	0.36
(1,2564)	1:393:A:GLN:HE22	1:474:A:GLU:HB2	4	0.36
(1,2564)	1:393:A:GLN:HE22	1:474:A:GLU:HB3	4	0.36
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	6	0.36
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	6	0.36
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	6	0.36
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	7	0.36
(1,2369)	1:380:A:LEU:HD11	1:463:A:ARG:H	15	0.36
(1,2369)	1:380:A:LEU:HD12	1:463:A:ARG:H	15	0.36
(1,2369)	1:380:A:LEU:HD13	1:463:A:ARG:H	15	0.36
(1,2367)	1:380:A:LEU:HD22	1:464:A:ILE:H	19	0.36
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE21	20	0.36
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE22	20	0.36
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE21	20	0.36
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE22	20	0.36
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	9	0.36
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	14	0.36
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	14	0.36
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	15	0.36
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	15	0.36
(1,2087)	1:362:A:LYS:HG2	1:366:A:ASP:H	5	0.36
(1,2087)	1:362:A:LYS:HG3	1:366:A:ASP:H	5	0.36
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	3	0.36
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD2	10	0.36
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD3	10	0.36
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	8	0.36
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	8	0.36
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	17	0.36
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	17	0.36
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	11	0.36
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	16	0.36
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	2	0.36
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	2	0.36
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	2	0.36
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	1	0.36
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	1	0.36
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	1	0.36
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	1	0.36
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	1	0.36
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	20	0.36
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	20	0.36
(1,1333)	1:303:A:ARG:H	1:327:A:SER:H	2	0.36
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	17	0.36
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	17	0.36
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	17	0.36
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	4	0.36
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	7	0.36
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	7	0.36
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	20	0.36
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	20	0.36
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	12	0.36
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	12	0.36
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	12	0.36
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	12	0.36
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	12	0.36
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	12	0.36
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	9	0.36
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	9	0.36
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	9	0.36
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	3	0.36
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	3	0.36
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	3	0.36
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	12	0.36
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	12	0.36
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	12	0.36
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	15	0.36
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	15	0.36
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	6	0.36
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	6	0.36
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	6	0.36
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	6	0.36
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	8	0.36
(1,266)	1:247:A:LYS:HE2	1:263:A:TRP:HH2	7	0.36
(1,266)	1:247:A:LYS:HE3	1:263:A:TRP:HH2	7	0.36
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	18	0.36
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	8	0.35
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	8	0.35
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	5	0.35
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	5	0.35
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	5	0.35
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	5	0.35
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	5	0.35
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	5	0.35
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	5	0.35
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	5	0.35
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	5	0.35
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	18	0.35
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	18	0.35
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	18	0.35
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	7	0.35
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	7	0.35
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	7	0.35
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	17	0.35
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	17	0.35
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	17	0.35
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	17	0.35
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	17	0.35
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	17	0.35
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	17	0.35
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	17	0.35
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	17	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	1	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	1	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	1	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	1	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	1	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	1	0.35
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	1	0.35
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	1	0.35
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	1	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	8	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	8	0.35
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	8	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	8	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	8	0.35
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	8	0.35
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	8	0.35
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	8	0.35
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	13	0.35
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	13	0.35
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	13	0.35
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	13	0.35
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	13	0.35
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	13	0.35
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	13	0.35
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	13	0.35
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	13	0.35
(1,3577)	1:473:A:THR:HA	1:479:A:PRO:HA	11	0.35
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	10	0.35
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	9	0.35
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	9	0.35
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	9	0.35
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB2	13	0.35
(1,3537)	1:469:A:MET:HE1	1:480:A:PHE:HB3	13	0.35
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB2	13	0.35
(1,3537)	1:469:A:MET:HE2	1:480:A:PHE:HB3	13	0.35
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB2	13	0.35
(1,3537)	1:469:A:MET:HE3	1:480:A:PHE:HB3	13	0.35
(1,3525)	1:468:A:MET:HA	1:472:A:LEU:H	14	0.35
(1,3385)	1:450:A:LEU:HA	1:455:A:ILE:HB	6	0.35
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	2	0.35
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	2	0.35
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	2	0.35
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	1	0.35
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	1	0.35
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB2	8	0.35
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB3	8	0.35
(1,3220)	1:436:A:ASP:HA	1:463:A:ARG:HA	20	0.35
(1,3200)	1:434:A:THR:HA	1:461:A:SER:HA	11	0.35
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	18	0.35
(1,3128)	1:430:A:ILE:HD11	1:474:A:GLU:HA	1	0.35
(1,3128)	1:430:A:ILE:HD12	1:474:A:GLU:HA	1	0.35
(1,3128)	1:430:A:ILE:HD13	1:474:A:GLU:HA	1	0.35
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	10	0.35
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	11	0.35
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	11	0.35
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	11	0.35
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	6	0.35
(1,2799)	1:405:A:THR:HB	1:456:A:GLU:HA	5	0.35
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	4	0.35
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	1	0.35
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	1	0.35
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	1	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	1	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	1	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	1	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	3	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	3	0.35
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	3	0.35
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	9	0.35
(1,2697)	1:402:A:PHE:HD1	1:461:A:SER:H	4	0.35
(1,2697)	1:402:A:PHE:HD2	1:461:A:SER:H	4	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	5	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	5	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	5	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	15	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	15	0.35
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	15	0.35
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	5	0.35
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	10	0.35
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	19	0.35
(1,2369)	1:380:A:LEU:HD11	1:463:A:ARG:H	14	0.35
(1,2369)	1:380:A:LEU:HD12	1:463:A:ARG:H	14	0.35
(1,2369)	1:380:A:LEU:HD13	1:463:A:ARG:H	14	0.35
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE21	11	0.35
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE22	11	0.35
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	13	0.35
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB1	15	0.35
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB2	15	0.35
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB3	15	0.35
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB1	15	0.35
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB2	15	0.35
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB3	15	0.35
(1,2070)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	3	0.35
(1,2070)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	3	0.35
(1,2070)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	3	0.35
(1,2070)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	3	0.35
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	16	0.35
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	10	0.35
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	17	0.35
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	3	0.35
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	10	0.35
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	17	0.35
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	17	0.35
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	17	0.35
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	17	0.35
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	17	0.35
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	17	0.35
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	17	0.35
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	17	0.35
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	17	0.35
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	15	0.35
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	15	0.35
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	17	0.35
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	17	0.35
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	10	0.35
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	10	0.35
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	10	0.35
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	10	0.35
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	12	0.35
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	12	0.35
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	12	0.35
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	12	0.35
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	4	0.35
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	4	0.35
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	14	0.35
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	14	0.35
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	19	0.35
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	10	0.35
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	10	0.35
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	10	0.35
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	5	0.35
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	5	0.35
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	15	0.35
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	15	0.35
(1,1021)	1:289:A:TRP:HH2	1:381:A:VAL:H	2	0.35
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD11	10	0.35
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD12	10	0.35
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD13	10	0.35
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	5	0.35
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	9	0.35
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	9	0.35
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	4	0.35
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	14	0.35
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	14	0.35
(1,668)	1:269:A:GLU:HA	1:273:A:GLU:HB2	7	0.35
(1,668)	1:269:A:GLU:HA	1:273:A:GLU:HB3	7	0.35
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	14	0.35
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	14	0.35
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	14	0.35
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	16	0.35
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	16	0.35
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	16	0.35
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	12	0.35
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	12	0.35
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	1	0.35
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	11	0.35
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	13	0.35
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	16	0.35
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	18	0.35
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	19	0.35
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	8	0.34
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	8	0.34
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	8	0.34
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	8	0.34
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	8	0.34
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	8	0.34
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	8	0.34
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	8	0.34
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	8	0.34
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	2	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	1	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	1	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	1	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	8	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	8	0.34
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	8	0.34
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	12	0.34
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	12	0.34
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	12	0.34
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	12	0.34
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	12	0.34
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	1	0.34
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	1	0.34
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	1	0.34
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	1	0.34
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	1	0.34
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	1	0.34
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	1	0.34
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	1	0.34
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	1	0.34
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	9	0.34
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	9	0.34
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	9	0.34
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	9	0.34
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	9	0.34
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	9	0.34
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	9	0.34
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	9	0.34
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	9	0.34
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	11	0.34
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	11	0.34
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	13	0.34
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	17	0.34
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB2	6	0.34
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB3	6	0.34
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	4	0.34
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	4	0.34
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	4	0.34
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	6	0.34
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	4	0.34
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	18	0.34
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	1	0.34
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	1	0.34
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	1	0.34
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	1	0.34
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	20	0.34
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	20	0.34
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	20	0.34
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	20	0.34
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG2	10	0.34
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG3	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG2	10	0.34
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG3	10	0.34
(1,3098)	1:429:A:LYS:HA	1:479:A:PRO:HG2	13	0.34
(1,3098)	1:429:A:LYS:HA	1:479:A:PRO:HG3	13	0.34
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	3	0.34
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	3	0.34
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	3	0.34
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	3	0.34
(1,3062)	1:426:A:GLY:HA2	1:428:A:GLU:HA	14	0.34
(1,3062)	1:426:A:GLY:HA3	1:428:A:GLU:HA	14	0.34
(1,3030)	1:423:A:MET:HE1	1:428:A:GLU:H	19	0.34
(1,3030)	1:423:A:MET:HE2	1:428:A:GLU:H	19	0.34
(1,3030)	1:423:A:MET:HE3	1:428:A:GLU:H	19	0.34
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	2	0.34
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	2	0.34
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	2	0.34
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	10	0.34
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	10	0.34
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	10	0.34
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	16	0.34
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	16	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	14	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	14	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	14	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	17	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	17	0.34
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	17	0.34
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	10	0.34
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	10	0.34
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	10	0.34
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	13	0.34
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	13	0.34
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	13	0.34
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	5	0.34
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	5	0.34
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	5	0.34
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	5	0.34
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	8	0.34
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	8	0.34
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	5	0.34
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	5	0.34
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	5	0.34
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	12	0.34
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	12	0.34
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	12	0.34
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	12	0.34
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	18	0.34
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	18	0.34
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	18	0.34
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD11	1	0.34
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD12	1	0.34
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD13	1	0.34
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	3	0.34
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	1	0.34
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	1	0.34
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	1	0.34
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	1	0.34
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	13	0.34
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	13	0.34
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	13	0.34
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	13	0.34
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	13	0.34
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	13	0.34
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	12	0.34
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	12	0.34
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	11	0.34
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	11	0.34
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	11	0.34
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	11	0.34
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	9	0.34
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	14	0.34
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	14	0.34
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	14	0.34
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD2	3	0.34
(1,1914)	1:351:A:ALA:HA	1:355:A:ARG:HD3	3	0.34
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	12	0.34
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	18	0.34
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	18	0.34
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	19	0.34
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	19	0.34
(1,1829)	1:344:A:VAL:HB	1:348:A:LEU:H	16	0.34
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	13	0.34
(1,1780)	1:339:A:LEU:HA	1:345:A:THR:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	1	0.34
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	1	0.34
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	8	0.34
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	8	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	9	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	9	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	9	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	9	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	9	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	9	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	9	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	9	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	9	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	20	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	20	0.34
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	20	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	20	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	20	0.34
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	20	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	20	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	20	0.34
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	20	0.34
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG2	18	0.34
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG3	18	0.34
(1,1556)	1:318:A:LEU:HD11	1:357:A:LEU:H	3	0.34
(1,1556)	1:318:A:LEU:HD12	1:357:A:LEU:H	3	0.34
(1,1556)	1:318:A:LEU:HD13	1:357:A:LEU:H	3	0.34
(1,1533)	1:317:A:TYR:HB2	1:385:A:GLY:H	3	0.34
(1,1533)	1:317:A:TYR:HB3	1:385:A:GLY:H	3	0.34
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	8	0.34
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	8	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	13	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	13	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	13	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	13	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	15	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	15	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	15	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	15	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	18	0.34
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	18	0.34
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	18	0.34
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	5	0.34
(1,1429)	1:312:A:GLN:HE21	1:336:A:ARG:HA	17	0.34
(1,1429)	1:312:A:GLN:HE22	1:336:A:ARG:HA	17	0.34
(1,1155)	1:298:A:LYS:H	1:323:A:GLY:H	13	0.34
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD2	2	0.34
(1,1117)	1:297:A:LEU:HA	1:322:A:ARG:HD3	2	0.34
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	10	0.34
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	10	0.34
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	12	0.34
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	3	0.34
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	2	0.34
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	2	0.34
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	2	0.34
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	2	0.34
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	4	0.34
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	4	0.34
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	4	0.34
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	12	0.34
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	12	0.34
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	20	0.34
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	11	0.34
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	11	0.34
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	11	0.34
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	11	0.34
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	11	0.34
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	11	0.34
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	7	0.34
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	2	0.34
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	2	0.34
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	2	0.34
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	2	0.34
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	16	0.34
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	16	0.34
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	16	0.34
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	2	0.34
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	2	0.34
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	2	0.34
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	8	0.34
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	8	0.34
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	8	0.34
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	2	0.33
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	2	0.33
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	2	0.33
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	2	0.33
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	2	0.33
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	2	0.33
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	2	0.33
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	2	0.33
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	2	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	5	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	5	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	5	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	6	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	6	0.33
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	6	0.33
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	1	0.33
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	1	0.33
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	1	0.33
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	1	0.33
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	14	0.33
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	14	0.33
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	14	0.33
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	14	0.33
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	14	0.33
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	14	0.33
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	14	0.33
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	14	0.33
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	14	0.33
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	15	0.33
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	15	0.33
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	15	0.33
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	15	0.33
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	15	0.33
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	15	0.33
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	15	0.33
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	15	0.33
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	15	0.33
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	1	0.33
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	1	0.33
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	1	0.33
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	1	0.33
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	1	0.33
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	1	0.33
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	1	0.33
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	1	0.33
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	18	0.33
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	18	0.33
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	18	0.33
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	18	0.33
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	18	0.33
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	18	0.33
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	18	0.33
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	18	0.33
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	18	0.33
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	11	0.33
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	11	0.33
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	11	0.33
(1,3507)	1:466:A:GLU:H	1:469:A:MET:H	8	0.33
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	2	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	3	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	3	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	3	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	17	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	17	0.33
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	17	0.33
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	12	0.33
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	12	0.33
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	12	0.33
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	14	0.33
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	14	0.33
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	14	0.33
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB2	10	0.33
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB3	10	0.33
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	3	0.33
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	11	0.33
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	10	0.33
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	10	0.33
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	10	0.33
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	3	0.33
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	3	0.33
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	3	0.33
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	3	0.33
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	12	0.33
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	12	0.33
(1,3075)	1:427:A:GLN:HG2	1:429:A:LYS:H	5	0.33
(1,3075)	1:427:A:GLN:HG3	1:429:A:LYS:H	5	0.33
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	3	0.33
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	3	0.33
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	5	0.33
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	5	0.33
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG2	13	0.33
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG3	13	0.33
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG2	13	0.33
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG3	13	0.33
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG2	13	0.33
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG3	13	0.33
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB2	4	0.33
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB3	4	0.33
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	17	0.33
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	17	0.33
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	19	0.33
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	19	0.33
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	19	0.33
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	13	0.33
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	13	0.33
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	13	0.33
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	11	0.33
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	8	0.33
(1,2712)	1:402:A:PHE:H	1:413:A:THR:H	20	0.33
(1,2590)	1:394:A:GLU:HA	1:397:A:ALA:H	20	0.33
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	3	0.33
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	11	0.33
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	1	0.33
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	7	0.33
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	6	0.33
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	20	0.33
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	4	0.33
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	4	0.33
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	9	0.33
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	9	0.33
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	19	0.33
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	15	0.33
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	20	0.33
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	20	0.33
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	20	0.33
(1,2040)	1:360:A:LEU:HD21	1:374:A:PHE:HD1	4	0.33
(1,2040)	1:360:A:LEU:HD21	1:374:A:PHE:HD2	4	0.33
(1,2040)	1:360:A:LEU:HD22	1:374:A:PHE:HD1	4	0.33
(1,2040)	1:360:A:LEU:HD22	1:374:A:PHE:HD2	4	0.33
(1,2040)	1:360:A:LEU:HD23	1:374:A:PHE:HD1	4	0.33
(1,2040)	1:360:A:LEU:HD23	1:374:A:PHE:HD2	4	0.33
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	17	0.33
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	17	0.33
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	17	0.33
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	17	0.33
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	17	0.33
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	17	0.33
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	20	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	2	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	2	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	2	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	2	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	2	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	2	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	2	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	2	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	2	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	18	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	18	0.33
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	18	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	18	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	18	0.33
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	18	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	18	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	18	0.33
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	18	0.33
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	11	0.33
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	11	0.33
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	9	0.33
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	9	0.33
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	9	0.33
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	9	0.33
(1,1487)	1:314:A:MET:HG2	1:319:A:ARG:HA	17	0.33
(1,1487)	1:314:A:MET:HG3	1:319:A:ARG:HA	17	0.33
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	1:314:A:MET:HA	1:353:A:THR:H	2	0.33
(1,1450)	1:313:A:PHE:HB2	1:348:A:LEU:HD11	19	0.33
(1,1450)	1:313:A:PHE:HB2	1:348:A:LEU:HD12	19	0.33
(1,1450)	1:313:A:PHE:HB2	1:348:A:LEU:HD13	19	0.33
(1,1450)	1:313:A:PHE:HB3	1:348:A:LEU:HD11	19	0.33
(1,1450)	1:313:A:PHE:HB3	1:348:A:LEU:HD12	19	0.33
(1,1450)	1:313:A:PHE:HB3	1:348:A:LEU:HD13	19	0.33
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	5	0.33
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	5	0.33
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	8	0.33
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	8	0.33
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	8	0.33
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	17	0.33
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	17	0.33
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	14	0.33
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	15	0.33
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	5	0.33
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	5	0.33
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	5	0.33
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	5	0.33
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	17	0.33
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	17	0.33
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	6	0.33
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	2	0.33
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	2	0.33
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	10	0.33
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	14	0.33
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	6	0.33
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	6	0.33
(1,927)	1:283:A:GLN:HA	1:377:A:GLN:HA	2	0.33
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	1	0.33
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	6	0.33
(1,850)	1:279:A:TYR:H	1:322:A:ARG:HB2	2	0.33
(1,850)	1:279:A:TYR:H	1:322:A:ARG:HB3	2	0.33
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	5	0.33
(1,708)	1:273:A:GLU:HB2	1:327:A:SER:HA	20	0.33
(1,708)	1:273:A:GLU:HB3	1:327:A:SER:HA	20	0.33
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	11	0.33
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	11	0.33
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	20	0.33
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	5	0.33
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	5	0.33
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	17	0.33
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	17	0.33
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	5	0.33
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	5	0.33
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	15	0.33
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	15	0.33
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	15	0.33
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	15	0.33
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	4	0.33
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	17	0.33
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	7	0.33
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	7	0.33
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	6	0.33
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	10	0.33
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	14	0.33
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	14	0.33
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	4	0.33
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	4	0.33
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	4	0.33
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	1	0.33
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	1	0.33
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	1	0.33
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	1	0.33
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	1	0.33
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	1	0.33
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	10	0.32
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	2	0.32
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	2	0.32
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	17	0.32
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	17	0.32
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	4	0.32
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	19	0.32
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	19	0.32
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	19	0.32
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	19	0.32
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	8	0.32
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	8	0.32
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	8	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	8	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	8	0.32
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	13	0.32
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	13	0.32
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	13	0.32
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	13	0.32
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	13	0.32
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	13	0.32
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	13	0.32
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	13	0.32
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	13	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	12	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	12	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	12	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	12	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	12	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	12	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	12	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	12	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	12	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	19	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	19	0.32
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	19	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	19	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	19	0.32
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	19	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	19	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	19	0.32
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	19	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	11	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	11	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	11	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	11	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	11	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	11	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	11	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	11	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	11	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	20	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	20	0.32
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	20	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	20	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	20	0.32
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	20	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	20	0.32
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	20	0.32
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	13	0.32
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	13	0.32
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	13	0.32
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	13	0.32
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	13	0.32
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	13	0.32
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	13	0.32
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	13	0.32
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	13	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	2	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	2	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	2	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	2	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	2	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	2	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	2	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	2	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	2	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	14	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	14	0.32
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	14	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	14	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	14	0.32
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	14	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	14	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	14	0.32
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	14	0.32
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	20	0.32
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	20	0.32
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	20	0.32
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	20	0.32
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	20	0.32
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	20	0.32
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	20	0.32
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	20	0.32
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	20	0.32
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE1	18	0.32
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE2	18	0.32
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE3	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE1	18	0.32
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE2	18	0.32
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE3	18	0.32
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE1	18	0.32
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE2	18	0.32
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE3	18	0.32
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB2	11	0.32
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB3	11	0.32
(1,3227)	1:437:A:SER:HA	1:461:A:SER:HA	7	0.32
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	6	0.32
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	7	0.32
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	7	0.32
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	7	0.32
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	7	0.32
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	7	0.32
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	7	0.32
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	7	0.32
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	18	0.32
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	18	0.32
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	18	0.32
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	15	0.32
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	15	0.32
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	15	0.32
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	15	0.32
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB2	11	0.32
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB3	11	0.32
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	3	0.32
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	15	0.32
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HE2	6	0.32
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	10	0.32
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	10	0.32
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	10	0.32
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	6	0.32
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	5	0.32
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	4	0.32
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	4	0.32
(1,2584)	1:394:A:GLU:HA	1:475:A:PHE:HA	20	0.32
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	11	0.32
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	11	0.32
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	11	0.32
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	14	0.32
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	14	0.32
(1,2492)	1:386:A:PRO:HG2	1:397:A:ALA:H	4	0.32
(1,2492)	1:386:A:PRO:HG3	1:397:A:ALA:H	4	0.32
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	3	0.32
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	3	0.32
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	3	0.32
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	3	0.32
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	3	0.32
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	3	0.32
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	13	0.32
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	2	0.32
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	12	0.32
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	12	0.32
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	4	0.32
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	4	0.32
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	4	0.32
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	4	0.32
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	4	0.32
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	4	0.32
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	6	0.32
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	6	0.32
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	6	0.32
(1,1926)	1:352:A:LEU:HD21	1:356:A:VAL:H	13	0.32
(1,1926)	1:352:A:LEU:HD22	1:356:A:VAL:H	13	0.32
(1,1926)	1:352:A:LEU:HD23	1:356:A:VAL:H	13	0.32
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	20	0.32
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	20	0.32
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	3	0.32
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	3	0.32
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	9	0.32
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	9	0.32
(1,1829)	1:344:A:VAL:HB	1:348:A:LEU:H	8	0.32
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	9	0.32
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	9	0.32
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	14	0.32
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	14	0.32
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	14	0.32
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	14	0.32
(1,1503)	1:315:A:PRO:HD2	1:350:A:ASN:HA	6	0.32
(1,1503)	1:315:A:PRO:HD3	1:350:A:ASN:HA	6	0.32
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	14	0.32
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	14	0.32
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	14	0.32
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	3	0.32
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	8	0.32
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	9	0.32
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	16	0.32
(1,1470)	1:314:A:MET:HA	1:353:A:THR:H	6	0.32
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	18	0.32
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	18	0.32
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	13	0.32
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	13	0.32
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	20	0.32
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	20	0.32
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	14	0.32
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	14	0.32
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	14	0.32
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	4	0.32
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	4	0.32
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	4	0.32
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	4	0.32
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	4	0.32
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	4	0.32
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	4	0.32
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	4	0.32
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	4	0.32
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	7	0.32
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	7	0.32
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	7	0.32
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	7	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	18	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	18	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	18	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	18	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	18	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	18	0.32
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	2	0.32
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	2	0.32
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	16	0.32
(1,672)	1:270:A:GLY:H	1:273:A:GLU:H	6	0.32
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	7	0.32
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	8	0.32
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	8	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	3	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	3	0.32
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	5	0.32
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	5	0.32
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	10	0.32
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	10	0.32
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	10	0.32
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	10	0.32
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	18	0.32
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	18	0.32
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	4	0.32
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	4	0.32
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	4	0.32
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	4	0.32
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	4	0.32
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	4	0.32
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	15	0.32
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	5	0.32
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	5	0.32
(1,339)	1:250:A:TYR:HE1	1:280:A:ILE:HA	18	0.32
(1,339)	1:250:A:TYR:HE2	1:280:A:ILE:HA	18	0.32
(1,267)	1:247:A:LYS:HG2	1:263:A:TRP:HH2	7	0.32
(1,267)	1:247:A:LYS:HG3	1:263:A:TRP:HH2	7	0.32
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	18	0.32
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	18	0.32
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	20	0.32
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	20	0.32
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	14	0.32
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	13	0.32
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	13	0.32
(1,135)	1:237:A:ASN:HD21	1:240:A:GLU:H	5	0.32
(1,135)	1:237:A:ASN:HD22	1:240:A:GLU:H	5	0.32
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	10	0.32
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	10	0.32
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	10	0.32
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	19	0.32
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	19	0.32
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	19	0.32
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	12	0.32
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	12	0.32
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	12	0.32
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	2	0.31
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	2	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	2	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	2	0.31
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	5	0.31
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	5	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	5	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	5	0.31
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	11	0.31
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	11	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	11	0.31
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	11	0.31
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	6	0.31
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	6	0.31
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	6	0.31
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	6	0.31
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	6	0.31
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	6	0.31
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	6	0.31
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	6	0.31
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	6	0.31
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	2	0.31
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	2	0.31
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	2	0.31
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	2	0.31
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	2	0.31
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	2	0.31
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	4	0.31
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	4	0.31
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	4	0.31
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	4	0.31
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	4	0.31
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	4	0.31
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	4	0.31
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	4	0.31
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	4	0.31
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	18	0.31
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	18	0.31
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	18	0.31
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	18	0.31
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	18	0.31
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	18	0.31
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	18	0.31
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	18	0.31
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	4	0.31
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	4	0.31
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	4	0.31
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	4	0.31
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	4	0.31
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	4	0.31
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	4	0.31
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	4	0.31
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	4	0.31
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	7	0.31
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	7	0.31
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	7	0.31
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	7	0.31
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	7	0.31
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	7	0.31
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	7	0.31
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	7	0.31
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	7	0.31
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	4	0.31
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	4	0.31
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	4	0.31
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	4	0.31
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	4	0.31
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	4	0.31
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	4	0.31
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	4	0.31
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	4	0.31
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	18	0.31
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	18	0.31
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	20	0.31
(1,3566)	1:472:A:LEU:HD21	1:475:A:PHE:HA	10	0.31
(1,3566)	1:472:A:LEU:HD22	1:475:A:PHE:HA	10	0.31
(1,3566)	1:472:A:LEU:HD23	1:475:A:PHE:HA	10	0.31
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD11	18	0.31
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD12	18	0.31
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD13	18	0.31
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD11	18	0.31
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD12	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD13	18	0.31
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD11	18	0.31
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD12	18	0.31
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD13	18	0.31
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	18	0.31
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	18	0.31
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	18	0.31
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB2	18	0.31
(1,3454)	1:460:A:LEU:HA	1:465:A:ASP:HB3	18	0.31
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	12	0.31
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	12	0.31
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	12	0.31
(1,3385)	1:450:A:LEU:HA	1:455:A:ILE:HB	17	0.31
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	11	0.31
(1,3372)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	11	0.31
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	11	0.31
(1,3372)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	11	0.31
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	11	0.31
(1,3372)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	11	0.31
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	11	0.31
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	11	0.31
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	11	0.31
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	11	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	7	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	7	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	7	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	18	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	18	0.31
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	18	0.31
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	11	0.31
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	11	0.31
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	11	0.31
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	17	0.31
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	17	0.31
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	17	0.31
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	13	0.31
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB2	8	0.31
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB3	8	0.31
(1,3180)	1:433:A:ILE:HA	1:482:A:SER:HB2	1	0.31
(1,3180)	1:433:A:ILE:HA	1:482:A:SER:HB3	1	0.31
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	6	0.31
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	6	0.31
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	6	0.31
(1,3096)	1:429:A:LYS:HB2	1:480:A:PHE:HA	12	0.31
(1,3096)	1:429:A:LYS:HB3	1:480:A:PHE:HA	12	0.31
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB2	5	0.31
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB3	5	0.31
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB2	5	0.31
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB3	5	0.31
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	1	0.31
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	12	0.31
(1,3044)	1:424:A:LYS:HE2	1:454:A:GLY:HA2	16	0.31
(1,3044)	1:424:A:LYS:HE2	1:454:A:GLY:HA3	16	0.31
(1,3044)	1:424:A:LYS:HE3	1:454:A:GLY:HA2	16	0.31
(1,3044)	1:424:A:LYS:HE3	1:454:A:GLY:HA3	16	0.31
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	2	0.31
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	2	0.31
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	2	0.31
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	19	0.31
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	19	0.31
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	19	0.31
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	2	0.31
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	2	0.31
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	2	0.31
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	2	0.31
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	2	0.31
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	2	0.31
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	17	0.31
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	5	0.31
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	5	0.31
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	1	0.31
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	1	0.31
(1,2836)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	10	0.31
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG2	16	0.31
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG3	16	0.31
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	12	0.31
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	20	0.31
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	12	0.31
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	12	0.31
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	12	0.31
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	19	0.31
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	15	0.31
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	2	0.31
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	2	0.31
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	2	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	10	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	10	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	10	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	13	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	13	0.31
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	13	0.31
(1,2712)	1:402:A:PHE:H	1:413:A:THR:H	18	0.31
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	2	0.31
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	2	0.31
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	2	0.31
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	3	0.31
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	3	0.31
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	16	0.31
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	16	0.31
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	4	0.31
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	4	0.31
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	4	0.31
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB2	2	0.31
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB3	2	0.31
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB2	2	0.31
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB3	2	0.31
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD11	15	0.31
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD12	15	0.31
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD13	15	0.31
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	11	0.31
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	3	0.31
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	3	0.31
(1,2369)	1:380:A:LEU:HD11	1:463:A:ARG:H	9	0.31
(1,2369)	1:380:A:LEU:HD12	1:463:A:ARG:H	9	0.31
(1,2369)	1:380:A:LEU:HD13	1:463:A:ARG:H	9	0.31
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	12	0.31
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	7	0.31
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	11	0.31
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	1	0.31
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	1	0.31
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	18	0.31
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	8	0.31
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	18	0.31
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	18	0.31
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	18	0.31
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	18	0.31
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	18	0.31
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	1	0.31
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	4	0.31
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	14	0.31
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	15	0.31
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	19	0.31
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	19	0.31
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	19	0.31
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	19	0.31
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	19	0.31
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	19	0.31
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	19	0.31
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	19	0.31
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	19	0.31
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	6	0.31
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	6	0.31
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	7	0.31
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	7	0.31
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	17	0.31
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	17	0.31
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	17	0.31
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	17	0.31
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	13	0.31
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	15	0.31
(1,1451)	1:313:A:PHE:HZ	1:345:A:THR:HA	13	0.31
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	11	0.31
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	11	0.31
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	11	0.31
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	11	0.31
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	11	0.31
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	11	0.31
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	13	0.31
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	13	0.31
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	10	0.31
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	10	0.31
(1,1323)	1:302:A:GLN:H	1:327:A:SER:H	2	0.31
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD11	2	0.31
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD12	2	0.31
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD13	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD11	2	0.31
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD12	2	0.31
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD13	2	0.31
(1,1076)	1:295:A:HIS:HB2	1:296:A:GLY:H	12	0.31
(1,1076)	1:295:A:HIS:HB3	1:296:A:GLY:H	12	0.31
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	19	0.31
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	14	0.31
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	14	0.31
(1,1066)	1:295:A:HIS:HB2	1:319:A:ARG:HA	15	0.31
(1,1066)	1:295:A:HIS:HB3	1:319:A:ARG:HA	15	0.31
(1,1023)	1:289:A:TRP:HH2	1:381:A:VAL:HA	3	0.31
(1,1021)	1:289:A:TRP:HH2	1:381:A:VAL:H	14	0.31
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	10	0.31
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	10	0.31
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	13	0.31
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	14	0.31
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	11	0.31
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	11	0.31
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	11	0.31
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	11	0.31
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	11	0.31
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	11	0.31
(1,851)	1:279:A:TYR:HB2	1:322:A:ARG:HB2	2	0.31
(1,851)	1:279:A:TYR:HB2	1:322:A:ARG:HB3	2	0.31
(1,851)	1:279:A:TYR:HB3	1:322:A:ARG:HB2	2	0.31
(1,851)	1:279:A:TYR:HB3	1:322:A:ARG:HB3	2	0.31
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	19	0.31
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	19	0.31
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	19	0.31
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	2	0.31
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	2	0.31
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	10	0.31
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	10	0.31
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	10	0.31
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	6	0.31
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	10	0.31
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	10	0.31
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	10	0.31
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	10	0.31
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	2	0.31
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	17	0.31
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	7	0.31
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	7	0.31
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	7	0.31
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	7	0.31
(1,266)	1:247:A:LYS:HE2	1:263:A:TRP:HH2	6	0.31
(1,266)	1:247:A:LYS:HE3	1:263:A:TRP:HH2	6	0.31
(1,225)	1:244:A:GLU:HA	1:247:A:LYS:HD2	14	0.31
(1,225)	1:244:A:GLU:HA	1:247:A:LYS:HD3	14	0.31
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	6	0.31
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	18	0.31
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	18	0.31
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	1	0.31
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	1	0.31
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	1	0.31
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	1	0.31
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	20	0.3
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	20	0.3
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	20	0.3
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	9	0.3
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	9	0.3
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	9	0.3
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	9	0.3
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	9	0.3
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	9	0.3
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	9	0.3
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	9	0.3
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	9	0.3
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	19	0.3
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	19	0.3
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	19	0.3
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	19	0.3
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	19	0.3
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	19	0.3
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	19	0.3
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	19	0.3
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	19	0.3
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	9	0.3
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	9	0.3
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	9	0.3
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	6	0.3
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	6	0.3
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	6	0.3
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	19	0.3
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	19	0.3
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	19	0.3
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	19	0.3
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	19	0.3
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	19	0.3
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	19	0.3
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	19	0.3
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	19	0.3
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	16	0.3
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	16	0.3
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	16	0.3
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	16	0.3
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	16	0.3
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	16	0.3
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	16	0.3
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	16	0.3
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	16	0.3
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	2	0.3
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	2	0.3
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	2	0.3
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	2	0.3
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	2	0.3
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	2	0.3
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	2	0.3
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	2	0.3
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	2	0.3
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	14	0.3
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	14	0.3
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	14	0.3
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	14	0.3
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	14	0.3
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	14	0.3
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	14	0.3
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	14	0.3
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	14	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	7	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	7	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	7	0.3
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	7	0.3
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	7	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	7	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	7	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	7	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	9	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	9	0.3
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	9	0.3
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	9	0.3
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	9	0.3
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	9	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	9	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	9	0.3
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	9	0.3
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	2	0.3
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	2	0.3
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	2	0.3
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	2	0.3
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	2	0.3
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	2	0.3
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	2	0.3
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	2	0.3
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	2	0.3
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	17	0.3
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	17	0.3
(1,3570)	1:472:A:LEU:HD21	1:474:A:GLU:HA	14	0.3
(1,3570)	1:472:A:LEU:HD22	1:474:A:GLU:HA	14	0.3
(1,3570)	1:472:A:LEU:HD23	1:474:A:GLU:HA	14	0.3
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	8	0.3
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	8	0.3
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	14	0.3
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	14	0.3
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	14	0.3
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	14	0.3
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	14	0.3
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	7	0.3
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	19	0.3
(1,3200)	1:434:A:THR:HA	1:461:A:SER:HA	14	0.3
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	13	0.3
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	13	0.3
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	13	0.3
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB2	2	0.3
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB3	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	18	0.3
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	11	0.3
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	18	0.3
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	18	0.3
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	18	0.3
(1,3030)	1:423:A:MET:HE1	1:428:A:GLU:H	17	0.3
(1,3030)	1:423:A:MET:HE2	1:428:A:GLU:H	17	0.3
(1,3030)	1:423:A:MET:HE3	1:428:A:GLU:H	17	0.3
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	20	0.3
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	20	0.3
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	20	0.3
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	20	0.3
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD2	9	0.3
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD3	9	0.3
(1,2887)	1:414:A:VAL:HG21	1:418:A:ASP:H	1	0.3
(1,2887)	1:414:A:VAL:HG22	1:418:A:ASP:H	1	0.3
(1,2887)	1:414:A:VAL:HG23	1:418:A:ASP:H	1	0.3
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	6	0.3
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	6	0.3
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD21	19	0.3
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD22	19	0.3
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD23	19	0.3
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	9	0.3
(1,2639)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	12	0.3
(1,2639)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	12	0.3
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	4	0.3
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	20	0.3
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	20	0.3
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	20	0.3
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	20	0.3
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	14	0.3
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD11	16	0.3
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD12	16	0.3
(1,2467)	1:385:A:GLY:H	1:396:A:ILE:HD13	16	0.3
(1,2454)	1:384:A:GLU:H	1:464:A:ILE:HD11	17	0.3
(1,2454)	1:384:A:GLU:H	1:464:A:ILE:HD12	17	0.3
(1,2454)	1:384:A:GLU:H	1:464:A:ILE:HD13	17	0.3
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	13	0.3
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE21	11	0.3
(1,2352)	1:379:A:GLY:HA2	1:412:A:GLN:HE22	11	0.3
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE21	11	0.3
(1,2352)	1:379:A:GLY:HA3	1:412:A:GLN:HE22	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	18	0.3
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	1	0.3
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	1	0.3
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	1	0.3
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	1	0.3
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	1	0.3
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	1	0.3
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	18	0.3
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	18	0.3
(1,2277)	1:375:A:TRP:HZ2	1:468:A:MET:HE1	12	0.3
(1,2277)	1:375:A:TRP:HZ2	1:468:A:MET:HE2	12	0.3
(1,2277)	1:375:A:TRP:HZ2	1:468:A:MET:HE3	12	0.3
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	8	0.3
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	8	0.3
(1,2207)	1:371:A:TYR:HD2	1:375:A:TRP:H	2	0.3
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	8	0.3
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	8	0.3
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	8	0.3
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	8	0.3
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	1	0.3
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	1	0.3
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	5	0.3
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	5	0.3
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB2	8	0.3
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB3	8	0.3
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	2	0.3
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	2	0.3
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	20	0.3
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	20	0.3
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	10	0.3
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	2	0.3
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	2	0.3
(1,1829)	1:344:A:VAL:HB	1:348:A:LEU:H	18	0.3
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE1	12	0.3
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE2	12	0.3
(1,1541)	1:317:A:TYR:HA	1:320:A:PHE:HD1	17	0.3
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	15	0.3
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	15	0.3
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	4	0.3
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	4	0.3
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	3	0.3
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	3	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	3	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	3	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	3	0.3
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	20	0.3
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	20	0.3
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	20	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	20	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	20	0.3
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	20	0.3
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB2	13	0.3
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB3	13	0.3
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB2	13	0.3
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB3	13	0.3
(1,1096)	1:296:A:GLY:H	1:309:A:ASP:HA	4	0.3
(1,1096)	1:296:A:GLY:H	1:309:A:ASP:HA	20	0.3
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	9	0.3
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	9	0.3
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	16	0.3
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	5	0.3
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	5	0.3
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	5	0.3
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	5	0.3
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	5	0.3
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	5	0.3
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	20	0.3
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	20	0.3
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	20	0.3
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	20	0.3
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	20	0.3
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	20	0.3
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	3	0.3
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	3	0.3
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	12	0.3
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	17	0.3
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	4	0.3
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	4	0.3
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	4	0.3
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	12	0.3
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	12	0.3
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD11	4	0.3
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD12	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD13	4	0.3
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD11	4	0.3
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD12	4	0.3
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD13	4	0.3
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	3	0.3
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	16	0.3
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	16	0.3
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	20	0.3
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB2	7	0.3
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB3	7	0.3
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	11	0.3
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	11	0.3
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	8	0.3
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	8	0.3
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	16	0.3
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	16	0.3
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	17	0.3
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	17	0.3
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	1	0.3
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	20	0.3
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	20	0.3
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	14	0.3
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	14	0.3
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	14	0.3
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	14	0.3
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	11	0.3
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	8	0.3
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	8	0.3
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	9	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	9	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	9	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	9	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	9	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	9	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	9	0.3
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	11	0.3
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	11	0.3
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	20	0.29
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	20	0.29
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	13	0.29
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	13	0.29
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	8	0.29
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	8	0.29
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	8	0.29
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	8	0.29
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	8	0.29
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	8	0.29
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	8	0.29
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	8	0.29
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	8	0.29
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	4	0.29
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	4	0.29
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	4	0.29
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	4	0.29
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	4	0.29
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	4	0.29
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	4	0.29
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	4	0.29
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	4	0.29
(1,3525)	1:468:A:MET:HA	1:472:A:LEU:H	4	0.29
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	8	0.29
(1,3469)	1:462:A:ASP:HB2	1:464:A:ILE:H	7	0.29
(1,3469)	1:462:A:ASP:HB3	1:464:A:ILE:H	7	0.29
(1,3469)	1:462:A:ASP:HB2	1:464:A:ILE:H	15	0.29
(1,3469)	1:462:A:ASP:HB3	1:464:A:ILE:H	15	0.29
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	18	0.29
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	18	0.29
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	18	0.29
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	16	0.29
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	16	0.29
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	16	0.29
(1,3317)	1:444:A:SER:H	1:447:A:LEU:H	10	0.29
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	2	0.29
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	2	0.29
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	11	0.29
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	11	0.29
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	7	0.29
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	9	0.29
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	9	0.29
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	17	0.29
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	17	0.29
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	9	0.29
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	13	0.29
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	13	0.29
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	13	0.29
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	13	0.29
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	14	0.29
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	14	0.29
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	14	0.29
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	14	0.29
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	18	0.29
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	18	0.29
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	8	0.29
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	5	0.29
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	5	0.29
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	5	0.29
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	8	0.29
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	8	0.29
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	8	0.29
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB2	16	0.29
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB3	16	0.29
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	5	0.29
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	5	0.29
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	5	0.29
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	5	0.29
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	7	0.29
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	7	0.29
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	15	0.29
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	15	0.29
(1,3022)	1:423:A:MET:HA	1:456:A:GLU:H	7	0.29
(1,3022)	1:423:A:MET:HA	1:456:A:GLU:H	10	0.29
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	14	0.29
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	14	0.29
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	6	0.29
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	11	0.29
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	18	0.29
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	18	0.29
(1,2836)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	6	0.29
(1,2827)	1:407:A:THR:H	1:409:A:SER:H	12	0.29
(1,2758)	1:404:A:SER:HB2	1:458:A:LEU:HA	18	0.29
(1,2758)	1:404:A:SER:HB3	1:458:A:LEU:HA	18	0.29
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	3	0.29
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	3	0.29
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2707)	1:402:A:PHE:HB2	1:415:A:SER:HA	16	0.29
(1,2707)	1:402:A:PHE:HB3	1:415:A:SER:HA	16	0.29
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	8	0.29
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	8	0.29
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	8	0.29
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	4	0.29
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	4	0.29
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	4	0.29
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	4	0.29
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	15	0.29
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	15	0.29
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	9	0.29
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	9	0.29
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	4	0.29
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	13	0.29
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	19	0.29
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB2	8	0.29
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB3	8	0.29
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB2	8	0.29
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB3	8	0.29
(1,2373)	1:380:A:LEU:HD21	1:412:A:GLN:HE21	20	0.29
(1,2373)	1:380:A:LEU:HD21	1:412:A:GLN:HE22	20	0.29
(1,2373)	1:380:A:LEU:HD22	1:412:A:GLN:HE21	20	0.29
(1,2373)	1:380:A:LEU:HD22	1:412:A:GLN:HE22	20	0.29
(1,2373)	1:380:A:LEU:HD23	1:412:A:GLN:HE21	20	0.29
(1,2373)	1:380:A:LEU:HD23	1:412:A:GLN:HE22	20	0.29
(1,2366)	1:380:A:LEU:HB2	1:464:A:ILE:H	5	0.29
(1,2366)	1:380:A:LEU:HB3	1:464:A:ILE:H	5	0.29
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	5	0.29
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	5	0.29
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	5	0.29
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	5	0.29
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	16	0.29
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	1	0.29
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	1	0.29
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	11	0.29
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	20	0.29
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	9	0.29
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	7	0.29
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	7	0.29
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	7	0.29
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	7	0.29
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	7	0.29
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	10	0.29
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	10	0.29
(1,1644)	1:325:A:ILE:HD11	1:327:A:SER:H	8	0.29
(1,1644)	1:325:A:ILE:HD12	1:327:A:SER:H	8	0.29
(1,1644)	1:325:A:ILE:HD13	1:327:A:SER:H	8	0.29
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	18	0.29
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	9	0.29
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	9	0.29
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	1	0.29
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	1	0.29
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	6	0.29
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	6	0.29
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	6	0.29
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	6	0.29
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	18	0.29
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	18	0.29
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	18	0.29
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	18	0.29
(1,1477)	1:314:A:MET:HE1	1:349:A:ARG:HA	16	0.29
(1,1477)	1:314:A:MET:HE2	1:349:A:ARG:HA	16	0.29
(1,1477)	1:314:A:MET:HE3	1:349:A:ARG:HA	16	0.29
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	7	0.29
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	7	0.29
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	7	0.29
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	7	0.29
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	7	0.29
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	7	0.29
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD11	12	0.29
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD12	12	0.29
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD13	12	0.29
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	7	0.29
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	7	0.29
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	20	0.29
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	20	0.29
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	20	0.29
(1,1316)	1:302:A:GLN:HE21	1:332:A:LEU:HD21	8	0.29
(1,1316)	1:302:A:GLN:HE21	1:332:A:LEU:HD22	8	0.29
(1,1316)	1:302:A:GLN:HE21	1:332:A:LEU:HD23	8	0.29
(1,1316)	1:302:A:GLN:HE22	1:332:A:LEU:HD21	8	0.29
(1,1316)	1:302:A:GLN:HE22	1:332:A:LEU:HD22	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1316)	1:302:A:GLN:HE22	1:332:A:LEU:HD23	8	0.29
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	5	0.29
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	5	0.29
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	4	0.29
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	4	0.29
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	4	0.29
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:HB	18	0.29
(1,1129)	1:297:A:LEU:H	1:311:A:GLU:HA	3	0.29
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	2	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	1	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	1	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	12	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	12	0.29
(1,1068)	1:295:A:HIS:HE1	1:316:A:ASN:HA	7	0.29
(1,1068)	1:295:A:HIS:HE1	1:316:A:ASN:HA	15	0.29
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	13	0.29
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	13	0.29
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	20	0.29
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	20	0.29
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	19	0.29
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	5	0.29
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	5	0.29
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	15	0.29
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	15	0.29
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	5	0.29
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	7	0.29
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	20	0.29
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	16	0.29
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	9	0.29
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	9	0.29
(1,571)	1:264:A:SER:HB2	1:359:A:MET:HB2	12	0.29
(1,571)	1:264:A:SER:HB2	1:359:A:MET:HB3	12	0.29
(1,571)	1:264:A:SER:HB3	1:359:A:MET:HB2	12	0.29
(1,571)	1:264:A:SER:HB3	1:359:A:MET:HB3	12	0.29
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	5	0.29
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	5	0.29
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	5	0.29
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	5	0.29
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	14	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	6	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	6	0.29
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	6	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	6	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	6	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	20	0.29
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	20	0.29
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	20	0.29
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	20	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	20	0.29
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	20	0.29
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	4	0.29
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	1	0.29
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	1	0.29
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	1	0.29
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	1	0.29
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	5	0.29
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	10	0.29
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	17	0.29
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	4	0.29
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD21	18	0.29
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD22	18	0.29
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD21	18	0.29
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD22	18	0.29
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	8	0.29
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	1	0.29
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	8	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	17	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	17	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	17	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	17	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	17	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	17	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	18	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	18	0.29
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	18	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	18	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	18	0.29
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	18	0.29
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	3	0.29
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	3	0.29
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	3	0.29
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	3	0.29
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	5	0.28
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	5	0.28
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	5	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	5	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	5	0.28
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	5	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	5	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	5	0.28
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	5	0.28
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	4	0.28
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	4	0.28
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	4	0.28
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	14	0.28
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	14	0.28
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	14	0.28
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	14	0.28
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	20	0.28
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	20	0.28
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	20	0.28
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	20	0.28
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	1	0.28
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	1	0.28
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	1	0.28
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	1	0.28
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	1	0.28
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	1	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	8	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	8	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	8	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	8	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	8	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	8	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	8	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	8	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	8	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	10	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	10	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	10	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	10	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	10	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	10	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	10	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	10	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	11	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	11	0.28
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	11	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	11	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	11	0.28
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	11	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	11	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	11	0.28
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	11	0.28
(1,3667)	1:434:A:THR:HG21	2:618:B:MET:HE1	18	0.28
(1,3667)	1:434:A:THR:HG21	2:618:B:MET:HE2	18	0.28
(1,3667)	1:434:A:THR:HG21	2:618:B:MET:HE3	18	0.28
(1,3667)	1:434:A:THR:HG22	2:618:B:MET:HE1	18	0.28
(1,3667)	1:434:A:THR:HG22	2:618:B:MET:HE2	18	0.28
(1,3667)	1:434:A:THR:HG22	2:618:B:MET:HE3	18	0.28
(1,3667)	1:434:A:THR:HG23	2:618:B:MET:HE1	18	0.28
(1,3667)	1:434:A:THR:HG23	2:618:B:MET:HE2	18	0.28
(1,3667)	1:434:A:THR:HG23	2:618:B:MET:HE3	18	0.28
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	14	0.28
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	14	0.28
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	14	0.28
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	14	0.28
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	14	0.28
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	14	0.28
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	14	0.28
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	14	0.28
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	14	0.28
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	6	0.28
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	6	0.28
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	3	0.28
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	4	0.28
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	18	0.28
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD11	7	0.28
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD12	7	0.28
(1,3544)	1:469:A:MET:HE1	1:472:A:LEU:HD13	7	0.28
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD11	7	0.28
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD12	7	0.28
(1,3544)	1:469:A:MET:HE2	1:472:A:LEU:HD13	7	0.28
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD11	7	0.28
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD12	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3544)	1:469:A:MET:HE3	1:472:A:LEU:HD13	7	0.28
(1,3469)	1:462:A:ASP:HB2	1:464:A:ILE:H	4	0.28
(1,3469)	1:462:A:ASP:HB3	1:464:A:ILE:H	4	0.28
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	8	0.28
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	20	0.28
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	20	0.28
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	6	0.28
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	6	0.28
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	7	0.28
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	7	0.28
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	20	0.28
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	1	0.28
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	1	0.28
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	2	0.28
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	14	0.28
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	19	0.28
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	17	0.28
(1,3152)	1:431:A:TYR:HB2	1:456:A:GLU:H	4	0.28
(1,3152)	1:431:A:TYR:HB3	1:456:A:GLU:H	4	0.28
(1,3075)	1:427:A:GLN:HG2	1:429:A:LYS:H	13	0.28
(1,3075)	1:427:A:GLN:HG3	1:429:A:LYS:H	13	0.28
(1,3075)	1:427:A:GLN:HG2	1:429:A:LYS:H	14	0.28
(1,3075)	1:427:A:GLN:HG3	1:429:A:LYS:H	14	0.28
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB2	11	0.28
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB3	11	0.28
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB2	11	0.28
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB3	11	0.28
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB2	11	0.28
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB3	11	0.28
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	17	0.28
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	17	0.28
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	17	0.28
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	17	0.28
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	17	0.28
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	17	0.28
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	4	0.28
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	7	0.28
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	15	0.28
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	15	0.28
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	15	0.28
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	15	0.28
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	15	0.28
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	15	0.28
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	15	0.28
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	15	0.28
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	19	0.28
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	19	0.28
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	19	0.28
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	16	0.28
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	16	0.28
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	16	0.28
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	9	0.28
(1,2735)	1:403:A:ALA:HA	1:414:A:VAL:HB	7	0.28
(1,2712)	1:402:A:PHE:H	1:413:A:THR:H	8	0.28
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	19	0.28
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	4	0.28
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	4	0.28
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	4	0.28
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	13	0.28
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	13	0.28
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	1	0.28
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	9	0.28
(1,2584)	1:394:A:GLU:HA	1:475:A:PHE:HA	19	0.28
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	2	0.28
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	18	0.28
(1,2427)	1:383:A:LYS:HA	1:464:A:ILE:HD11	17	0.28
(1,2427)	1:383:A:LYS:HA	1:464:A:ILE:HD12	17	0.28
(1,2427)	1:383:A:LYS:HA	1:464:A:ILE:HD13	17	0.28
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	20	0.28
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	6	0.28
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	6	0.28
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE1	19	0.28
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE2	19	0.28
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE3	19	0.28
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	1	0.28
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	1	0.28
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	5	0.28
(1,2262)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	5	0.28
(1,2229)	1:372:A:GLN:HE21	1:376:A:GLN:H	4	0.28
(1,2229)	1:372:A:GLN:HE22	1:376:A:GLN:H	4	0.28
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	7	0.28
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	7	0.28
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	7	0.28
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	13	0.28
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	15	0.28
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	15	0.28
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	15	0.28
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	16	0.28
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	16	0.28
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	16	0.28
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	16	0.28
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	16	0.28
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	16	0.28
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	8	0.28
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	8	0.28
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	19	0.28
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	19	0.28
(1,1797)	1:340:A:GLN:HA	1:342:A:SER:H	16	0.28
(1,1747)	1:336:A:ARG:HG2	1:340:A:GLN:H	10	0.28
(1,1747)	1:336:A:ARG:HG3	1:340:A:GLN:H	10	0.28
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	3	0.28
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	3	0.28
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	3	0.28
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	3	0.28
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	3	0.28
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	3	0.28
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	3	0.28
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	3	0.28
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	3	0.28
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	10	0.28
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	10	0.28
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	9	0.28
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	9	0.28
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	18	0.28
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	18	0.28
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	19	0.28
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	19	0.28
(1,1487)	1:314:A:MET:HG2	1:319:A:ARG:HA	9	0.28
(1,1487)	1:314:A:MET:HG3	1:319:A:ARG:HA	9	0.28
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	19	0.28
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	19	0.28
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	14	0.28
(1,1470)	1:314:A:MET:HA	1:353:A:THR:H	5	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	4	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	4	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	4	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	4	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	4	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	13	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	13	0.28
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	13	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	13	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	13	0.28
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	13	0.28
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD11	8	0.28
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD12	8	0.28
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD13	8	0.28
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	15	0.28
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	15	0.28
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	15	0.28
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	15	0.28
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	15	0.28
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	2	0.28
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	2	0.28
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	2	0.28
(1,1320)	1:302:A:GLN:HA	1:328:A:SER:HA	1	0.28
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	12	0.28
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	12	0.28
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:HB	19	0.28
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	10	0.28
(1,1068)	1:295:A:HIS:HE1	1:316:A:ASN:HA	18	0.28
(1,1064)	1:295:A:HIS:HA	1:320:A:PHE:HA	2	0.28
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	19	0.28
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	19	0.28
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	19	0.28
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	19	0.28
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	12	0.28
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	12	0.28
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	18	0.28
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	18	0.28
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	18	0.28
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	3	0.28
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	3	0.28
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	3	0.28
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	3	0.28
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	3	0.28
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	19	0.28
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	15	0.28
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	15	0.28
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	8	0.28
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	3	0.28
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	19	0.28
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	19	0.28
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	3	0.28
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	11	0.28
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	11	0.28
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	12	0.28
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	18	0.28
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	18	0.28
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	1	0.28
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	1	0.28
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	18	0.28
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	18	0.28
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	18	0.28
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	18	0.28
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	18	0.28
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	18	0.28
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	9	0.28
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	1	0.28
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	18	0.28
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	17	0.28
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	8	0.28
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	1	0.28
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	5	0.28
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	3	0.28
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	10	0.28
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	17	0.28
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	19	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	2	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	2	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	2	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	2	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	2	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	2	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	4	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	4	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	4	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	4	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	4	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	19	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	19	0.28
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	19	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	19	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	19	0.28
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	19	0.28
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD2	3	0.28
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD3	3	0.28
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD2	3	0.28
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD3	3	0.28
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	7	0.28
(2,12)	1:419:A:TYR:HE2	1:478:A:LYS:HB2	20	0.27
(2,12)	1:419:A:TYR:HE2	1:478:A:LYS:HB3	20	0.27
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	15	0.27
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	15	0.27
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	15	0.27
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	14	0.27
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	14	0.27
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	14	0.27
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	6	0.27
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	6	0.27
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	6	0.27
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	6	0.27
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	6	0.27
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	6	0.27
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	6	0.27
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	6	0.27
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	6	0.27
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	6	0.27
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	6	0.27
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	6	0.27
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	6	0.27
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	6	0.27
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	6	0.27
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	8	0.27
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	8	0.27
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	8	0.27
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	8	0.27
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	8	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	8	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	8	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	8	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	8	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	8	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	8	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	8	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	8	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	8	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	14	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	14	0.27
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	14	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	14	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	14	0.27
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	14	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	14	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	14	0.27
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	14	0.27
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	11	0.27
(1,3582)	1:474:A:GLU:H	1:480:A:PHE:H	3	0.27
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	11	0.27
(1,3528)	1:468:A:MET:HA	1:471:A:TYR:H	2	0.27
(1,3487)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	3	0.27
(1,3487)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	3	0.27
(1,3487)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	3	0.27
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	16	0.27
(1,3469)	1:462:A:ASP:HB2	1:464:A:ILE:H	9	0.27
(1,3469)	1:462:A:ASP:HB3	1:464:A:ILE:H	9	0.27
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB2	6	0.27
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB3	6	0.27
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	9	0.27
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	9	0.27
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	9	0.27
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	9	0.27
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	9	0.27
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	9	0.27
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	3	0.27
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	7	0.27
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	13	0.27
(1,3363)	1:448:A:GLU:HA	1:451:A:ARG:H	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	2	0.27
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	2	0.27
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	20	0.27
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	20	0.27
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	20	0.27
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	12	0.27
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	12	0.27
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB2	9	0.27
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB3	9	0.27
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	3	0.27
(1,3152)	1:431:A:TYR:HB2	1:456:A:GLU:H	17	0.27
(1,3152)	1:431:A:TYR:HB3	1:456:A:GLU:H	17	0.27
(1,3136)	1:431:A:TYR:HA	1:482:A:SER:HA	11	0.27
(1,3136)	1:431:A:TYR:HA	1:482:A:SER:HA	17	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	14	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	14	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	14	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	15	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	15	0.27
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	15	0.27
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	19	0.27
(1,3067)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	19	0.27
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	19	0.27
(1,3067)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	19	0.27
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD2	8	0.27
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD3	8	0.27
(1,2950)	1:418:A:ASP:HA	1:421:A:SER:HB2	8	0.27
(1,2950)	1:418:A:ASP:HA	1:421:A:SER:HB3	8	0.27
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	19	0.27
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	19	0.27
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	10	0.27
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	10	0.27
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	1	0.27
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	2	0.27
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	20	0.27
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	20	0.27
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	20	0.27
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	15	0.27
(1,2639)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	17	0.27
(1,2639)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	17	0.27
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	7	0.27
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	6	0.27
(1,2584)	1:394:A:GLU:HA	1:475:A:PHE:HA	15	0.27
(1,2583)	1:394:A:GLU:HG2	1:476:A:ASP:H	6	0.27
(1,2583)	1:394:A:GLU:HG3	1:476:A:ASP:H	6	0.27
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	10	0.27
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	13	0.27
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	15	0.27
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	15	0.27
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	15	0.27
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	15	0.27
(1,2478)	1:386:A:PRO:HB2	1:472:A:LEU:HA	5	0.27
(1,2478)	1:386:A:PRO:HB3	1:472:A:LEU:HA	5	0.27
(1,2478)	1:386:A:PRO:HB2	1:472:A:LEU:HA	6	0.27
(1,2478)	1:386:A:PRO:HB3	1:472:A:LEU:HA	6	0.27
(1,2478)	1:386:A:PRO:HB2	1:472:A:LEU:HA	15	0.27
(1,2478)	1:386:A:PRO:HB3	1:472:A:LEU:HA	15	0.27
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	17	0.27
(1,2368)	1:380:A:LEU:HB2	1:464:A:ILE:HB	5	0.27
(1,2368)	1:380:A:LEU:HB3	1:464:A:ILE:HB	5	0.27
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	8	0.27
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	8	0.27
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	20	0.27
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	9	0.27
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	9	0.27
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	9	0.27
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	9	0.27
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB1	11	0.27
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB2	11	0.27
(1,2071)	1:361:A:GLU:HB2	1:395:A:ALA:HB3	11	0.27
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB1	11	0.27
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB2	11	0.27
(1,2071)	1:361:A:GLU:HB3	1:395:A:ALA:HB3	11	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	5	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	5	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	5	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	17	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	17	0.27
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	17	0.27
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	3	0.27
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	12	0.27
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	2	0.27
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	3	0.27
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	7	0.27
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	11	0.27
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB2	11	0.27
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB3	11	0.27
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB2	11	0.27
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB3	11	0.27
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	12	0.27
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	12	0.27
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	5	0.27
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	5	0.27
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	5	0.27
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	5	0.27
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	12	0.27
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	12	0.27
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	14	0.27
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	14	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	8	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	8	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	8	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	8	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	8	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	8	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	10	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	10	0.27
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	10	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	10	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	10	0.27
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	10	0.27
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	5	0.27
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	5	0.27
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	17	0.27
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	17	0.27
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	17	0.27
(1,1297)	1:301:A:VAL:H	1:306:A:ILE:HB	10	0.27
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	18	0.27
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	10	0.27
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	10	0.27
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	10	0.27
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	7	0.27
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	8	0.27
(1,1059)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	8	0.27
(1,1059)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	8	0.27
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	18	0.27
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	18	0.27
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	8	0.27
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	10	0.27
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	16	0.27
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HG21	14	0.27
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HG22	14	0.27
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HG23	14	0.27
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD21	19	0.27
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD22	19	0.27
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD23	19	0.27
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD21	19	0.27
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD22	19	0.27
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD23	19	0.27
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD21	19	0.27
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD22	19	0.27
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD23	19	0.27
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	15	0.27
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	18	0.27
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	18	0.27
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	11	0.27
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	7	0.27
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	7	0.27
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	6	0.27
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	6	0.27
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	15	0.27
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	15	0.27
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	4	0.27
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	4	0.27
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	6	0.27
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	6	0.27
(1,633)	1:267:A:ARG:HA	1:274:A:TYR:H	1	0.27
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	15	0.27
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	15	0.27
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	8	0.27
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	8	0.27
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	6	0.27
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	12	0.27
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	12	0.27
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	12	0.27
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	13	0.27
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	15	0.27
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	5	0.27
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	5	0.27
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	5	0.27
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	5	0.27
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	7	0.27
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	7	0.27
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	7	0.27
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	7	0.27
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD2	18	0.27
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD3	18	0.27
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD2	18	0.27
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD3	18	0.27
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	6	0.27
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	14	0.27
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	17	0.27
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	15	0.27
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	2	0.27
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	5	0.27
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	17	0.27
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	17	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	17	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	17	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	17	0.27
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	20	0.27
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	6	0.26
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	19	0.26
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	10	0.26
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	10	0.26
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	10	0.26
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	10	0.26
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	10	0.26
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	10	0.26
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	7	0.26
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	7	0.26
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	7	0.26
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	7	0.26
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	7	0.26
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	7	0.26
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	7	0.26
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	7	0.26
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	11	0.26
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	11	0.26
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	11	0.26
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	11	0.26
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	11	0.26
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	11	0.26
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	11	0.26
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	11	0.26
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	11	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	4	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	4	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	4	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	4	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	4	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	4	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	4	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	4	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	4	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	15	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	15	0.26
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	15	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	15	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	15	0.26
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	15	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	15	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	15	0.26
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	15	0.26
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	20	0.26
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	20	0.26
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	20	0.26
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	20	0.26
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	20	0.26
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	20	0.26
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	20	0.26
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	20	0.26
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	20	0.26
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	20	0.26
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	20	0.26
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	20	0.26
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	20	0.26
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	20	0.26
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	20	0.26
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	20	0.26
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	20	0.26
(1,3570)	1:472:A:LEU:HD21	1:474:A:GLU:HA	5	0.26
(1,3570)	1:472:A:LEU:HD22	1:474:A:GLU:HA	5	0.26
(1,3570)	1:472:A:LEU:HD23	1:474:A:GLU:HA	5	0.26
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	17	0.26
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	4	0.26
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	6	0.26
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE1	11	0.26
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE2	11	0.26
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE3	11	0.26
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE1	11	0.26
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE2	11	0.26
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE3	11	0.26
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE1	11	0.26
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE2	11	0.26
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE3	11	0.26
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	2	0.26
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	10	0.26
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	12	0.26
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	16	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG21	11	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG22	11	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG23	11	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG21	11	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG22	11	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG23	11	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG21	12	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG22	12	0.26
(1,3397)	1:451:A:ARG:HB2	1:457:A:VAL:HG23	12	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG21	12	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG22	12	0.26
(1,3397)	1:451:A:ARG:HB3	1:457:A:VAL:HG23	12	0.26
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	11	0.26
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	11	0.26
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	11	0.26
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	9	0.26
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	9	0.26
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	13	0.26
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	13	0.26
(1,3276)	1:440:A:ALA:HA	1:442:A:LYS:H	6	0.26
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	4	0.26
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB2	2	0.26
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB3	2	0.26
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	9	0.26
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	19	0.26
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	7	0.26
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	8	0.26
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	4	0.26
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	4	0.26
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	2	0.26
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	17	0.26
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	17	0.26
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	17	0.26
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	6	0.26
(1,3069)	1:427:A:GLN:HE21	1:455:A:ILE:HA	18	0.26
(1,3069)	1:427:A:GLN:HE22	1:455:A:ILE:HA	18	0.26
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	7	0.26
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	7	0.26
(1,3042)	1:424:A:LYS:HE2	1:455:A:ILE:HA	5	0.26
(1,3042)	1:424:A:LYS:HE3	1:455:A:ILE:HA	5	0.26
(1,3030)	1:423:A:MET:HE1	1:428:A:GLU:H	18	0.26
(1,3030)	1:423:A:MET:HE2	1:428:A:GLU:H	18	0.26
(1,3030)	1:423:A:MET:HE3	1:428:A:GLU:H	18	0.26
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	14	0.26
(1,2918)	1:416:A:LEU:HA	1:420:A:VAL:H	19	0.26
(1,2910)	1:416:A:LEU:HB2	1:475:A:PHE:HZ	10	0.26
(1,2910)	1:416:A:LEU:HB3	1:475:A:PHE:HZ	10	0.26
(1,2874)	1:412:A:GLN:HA	1:414:A:VAL:HB	9	0.26
(1,2849)	1:409:A:SER:H	1:411:A:ALA:H	17	0.26
(1,2827)	1:407:A:THR:H	1:409:A:SER:H	9	0.26
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	15	0.26
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	15	0.26
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	15	0.26
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	20	0.26
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	20	0.26
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	20	0.26
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	20	0.26
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	20	0.26
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	13	0.26
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	18	0.26
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	8	0.26
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	8	0.26
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	6	0.26
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	6	0.26
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	12	0.26
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	4	0.26
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	12	0.26
(1,2387)	1:381:A:VAL:HA	1:385:A:GLY:H	7	0.26
(1,2374)	1:380:A:LEU:HA	1:384:A:GLU:H	9	0.26
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB2	10	0.26
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB3	10	0.26
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB2	10	0.26
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB3	10	0.26
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB2	10	0.26
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB3	10	0.26
(1,2229)	1:372:A:GLN:HE21	1:376:A:GLN:H	18	0.26
(1,2229)	1:372:A:GLN:HE22	1:376:A:GLN:H	18	0.26
(1,2144)	1:365:A:LYS:HA	1:367:A:ASP:H	16	0.26
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	20	0.26
(1,2137)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	20	0.26
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	20	0.26
(1,2137)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	20	0.26
(1,2033)	1:360:A:LEU:HD11	1:399:A:LEU:HD11	7	0.26
(1,2033)	1:360:A:LEU:HD11	1:399:A:LEU:HD12	7	0.26
(1,2033)	1:360:A:LEU:HD11	1:399:A:LEU:HD13	7	0.26
(1,2033)	1:360:A:LEU:HD12	1:399:A:LEU:HD11	7	0.26
(1,2033)	1:360:A:LEU:HD12	1:399:A:LEU:HD12	7	0.26
(1,2033)	1:360:A:LEU:HD12	1:399:A:LEU:HD13	7	0.26
(1,2033)	1:360:A:LEU:HD13	1:399:A:LEU:HD11	7	0.26
(1,2033)	1:360:A:LEU:HD13	1:399:A:LEU:HD12	7	0.26
(1,2033)	1:360:A:LEU:HD13	1:399:A:LEU:HD13	7	0.26
(1,2009)	1:358:A:GLN:HA	1:361:A:GLU:H	9	0.26
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	4	0.26
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	9	0.26
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	15	0.26
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	8	0.26
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	7	0.26
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	13	0.26
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	8	0.26
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	15	0.26
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	15	0.26
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	15	0.26
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	18	0.26
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	18	0.26
(1,1828)	1:344:A:VAL:HA	1:348:A:LEU:H	16	0.26
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	2	0.26
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	13	0.26
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	13	0.26
(1,1503)	1:315:A:PRO:HD2	1:350:A:ASN:HA	3	0.26
(1,1503)	1:315:A:PRO:HD3	1:350:A:ASN:HA	3	0.26
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	3	0.26
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	3	0.26
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	6	0.26
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	6	0.26
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	9	0.26
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	9	0.26
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	12	0.26
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	12	0.26
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	15	0.26
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	15	0.26
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	7	0.26
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	7	0.26
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	7	0.26
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	16	0.26
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	16	0.26
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	16	0.26
(1,1276)	1:301:A:VAL:HB	1:332:A:LEU:HD11	6	0.26
(1,1276)	1:301:A:VAL:HB	1:332:A:LEU:HD12	6	0.26
(1,1276)	1:301:A:VAL:HB	1:332:A:LEU:HD13	6	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	3	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	3	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	17	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	17	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	19	0.26
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	19	0.26
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	20	0.26
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	15	0.26
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	19	0.26
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	19	0.26
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	9	0.26
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	3	0.26
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	3	0.26
(1,1021)	1:289:A:TRP:HH2	1:381:A:VAL:H	8	0.26
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	16	0.26
(1,964)	1:285:A:PRO:HG2	1:288:A:MET:HA	11	0.26
(1,964)	1:285:A:PRO:HG3	1:288:A:MET:HA	11	0.26
(1,936)	1:284:A:ALA:HA	1:378:A:PHE:HZ	15	0.26
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	4	0.26
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	17	0.26
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	17	0.26
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	3	0.26
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	10	0.26
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	2	0.26
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	2	0.26
(1,575)	1:264:A:SER:HB2	1:356:A:VAL:HA	11	0.26
(1,575)	1:264:A:SER:HB3	1:356:A:VAL:HA	11	0.26
(1,572)	1:264:A:SER:H	1:359:A:MET:HE1	20	0.26
(1,572)	1:264:A:SER:H	1:359:A:MET:HE2	20	0.26
(1,572)	1:264:A:SER:H	1:359:A:MET:HE3	20	0.26
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	8	0.26
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	1	0.26
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	1	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	1	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	1	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	1	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	1	0.26
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	3	0.26
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	3	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	3	0.26
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	3	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	3	0.26
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	3	0.26
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	9	0.26
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	12	0.26
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	8	0.26
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	11	0.26
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	11	0.26
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	17	0.26
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	17	0.26
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	3	0.26
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	4	0.26
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	2	0.26
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	2	0.26
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	2	0.26
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	8	0.25
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	18	0.25
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	18	0.25
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	18	0.25
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	18	0.25
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	18	0.25
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	18	0.25
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	18	0.25
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	18	0.25
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	18	0.25
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	18	0.25
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	20	0.25
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	6	0.25
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	6	0.25
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	6	0.25
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	17	0.25
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	17	0.25
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	17	0.25
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	17	0.25
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	17	0.25
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	17	0.25
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	17	0.25
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	17	0.25
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	17	0.25
(1,3666)	1:464:A:ILE:HD11	2:624:B:MET:HE1	5	0.25
(1,3666)	1:464:A:ILE:HD11	2:624:B:MET:HE2	5	0.25
(1,3666)	1:464:A:ILE:HD11	2:624:B:MET:HE3	5	0.25
(1,3666)	1:464:A:ILE:HD12	2:624:B:MET:HE1	5	0.25
(1,3666)	1:464:A:ILE:HD12	2:624:B:MET:HE2	5	0.25
(1,3666)	1:464:A:ILE:HD12	2:624:B:MET:HE3	5	0.25
(1,3666)	1:464:A:ILE:HD13	2:624:B:MET:HE1	5	0.25
(1,3666)	1:464:A:ILE:HD13	2:624:B:MET:HE2	5	0.25
(1,3666)	1:464:A:ILE:HD13	2:624:B:MET:HE3	5	0.25
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	20	0.25
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	20	0.25
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	20	0.25
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	20	0.25
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	20	0.25
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	20	0.25
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	20	0.25
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	20	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	6	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	6	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	6	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	6	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	6	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	6	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	6	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	6	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	6	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	9	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	9	0.25
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	9	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	9	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	9	0.25
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	9	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	9	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	9	0.25
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	9	0.25
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	19	0.25
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	19	0.25
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	19	0.25
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	19	0.25
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	19	0.25
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	19	0.25
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	19	0.25
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	19	0.25
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	19	0.25
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	5	0.25
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	7	0.25
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	7	0.25
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	7	0.25
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	7	0.25
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	19	0.25
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	4	0.25
(1,3363)	1:448:A:GLU:HA	1:451:A:ARG:H	5	0.25
(1,3348)	1:447:A:LEU:HA	1:451:A:ARG:H	19	0.25
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	8	0.25
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	8	0.25
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	12	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	12	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	12	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	16	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	16	0.25
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	16	0.25
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	10	0.25
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	10	0.25
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	14	0.25
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	14	0.25
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	13	0.25
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	18	0.25
(1,3249)	1:438:A:TYR:HE1	1:442:A:LYS:HD2	13	0.25
(1,3249)	1:438:A:TYR:HE1	1:442:A:LYS:HD3	13	0.25
(1,3249)	1:438:A:TYR:HE2	1:442:A:LYS:HD2	13	0.25
(1,3249)	1:438:A:TYR:HE2	1:442:A:LYS:HD3	13	0.25
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB2	15	0.25
(1,3199)	1:434:A:THR:HA	1:465:A:ASP:HB3	15	0.25
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	20	0.25
(1,3181)	1:433:A:ILE:H	1:460:A:LEU:H	15	0.25
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	3	0.25
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	3	0.25
(1,3111)	1:430:A:ILE:H	1:481:A:GLN:H	4	0.25
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	13	0.25
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	13	0.25
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	13	0.25
(1,3101)	1:429:A:LYS:HA	1:478:A:LYS:HA	20	0.25
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	16	0.25
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	16	0.25
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	16	0.25
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	16	0.25
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	11	0.25
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	11	0.25
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	2	0.25
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	4	0.25
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	11	0.25
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD11	9	0.25
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD12	9	0.25
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD13	9	0.25
(1,2827)	1:407:A:THR:H	1:409:A:SER:H	5	0.25
(1,2827)	1:407:A:THR:H	1:409:A:SER:H	16	0.25
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD21	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD22	9	0.25
(1,2791)	1:405:A:THR:H	1:458:A:LEU:HD23	9	0.25
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG11	20	0.25
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG12	20	0.25
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG13	20	0.25
(1,2764)	1:404:A:SER:HA	1:456:A:GLU:HG2	6	0.25
(1,2764)	1:404:A:SER:HA	1:456:A:GLU:HG3	6	0.25
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	19	0.25
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	7	0.25
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	20	0.25
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD11	17	0.25
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD12	17	0.25
(1,2648)	1:398:A:LYS:HA	1:416:A:LEU:HD13	17	0.25
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	15	0.25
(1,2529)	1:388:A:GLU:H	1:390:A:PHE:H	2	0.25
(1,2519)	1:387:A:ALA:HB1	1:467:A:TRP:HZ2	19	0.25
(1,2519)	1:387:A:ALA:HB2	1:467:A:TRP:HZ2	19	0.25
(1,2519)	1:387:A:ALA:HB3	1:467:A:TRP:HZ2	19	0.25
(1,2518)	1:387:A:ALA:HB1	1:467:A:TRP:HH2	19	0.25
(1,2518)	1:387:A:ALA:HB2	1:467:A:TRP:HH2	19	0.25
(1,2518)	1:387:A:ALA:HB3	1:467:A:TRP:HH2	19	0.25
(1,2375)	1:380:A:LEU:H	1:383:A:LYS:H	9	0.25
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	9	0.25
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	9	0.25
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	4	0.25
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	4	0.25
(1,2018)	1:359:A:MET:HG2	1:363:A:LEU:H	2	0.25
(1,2018)	1:359:A:MET:HG3	1:363:A:LEU:H	2	0.25
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	3	0.25
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	3	0.25
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	3	0.25
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	13	0.25
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	2	0.25
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	20	0.25
(1,1541)	1:317:A:TYR:HA	1:320:A:PHE:HD1	12	0.25
(1,1533)	1:317:A:TYR:HB2	1:385:A:GLY:H	13	0.25
(1,1533)	1:317:A:TYR:HB3	1:385:A:GLY:H	13	0.25
(1,1510)	1:315:A:PRO:HG2	1:318:A:LEU:H	16	0.25
(1,1510)	1:315:A:PRO:HG3	1:318:A:LEU:H	16	0.25
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	5	0.25
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	5	0.25
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	14	0.25
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	8	0.25
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	8	0.25
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	8	0.25
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	8	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	12	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	12	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	12	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	12	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	12	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	12	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	14	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	14	0.25
(1,1442)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	14	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	14	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	14	0.25
(1,1442)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	14	0.25
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB2	7	0.25
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HB3	7	0.25
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB2	7	0.25
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HB3	7	0.25
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	4	0.25
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	4	0.25
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	4	0.25
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	14	0.25
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	14	0.25
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	14	0.25
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	19	0.25
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	19	0.25
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	19	0.25
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	11	0.25
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	11	0.25
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	9	0.25
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	19	0.25
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	11	0.25
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	11	0.25
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	11	0.25
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	8	0.25
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	5	0.25
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	5	0.25
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	1	0.25
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	3	0.25
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD11	6	0.25
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD12	6	0.25
(1,1020)	1:289:A:TRP:HH2	1:464:A:ILE:HD13	6	0.25
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	4	0.25
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	19	0.25
(1,963)	1:285:A:PRO:HG2	1:288:A:MET:H	5	0.25
(1,963)	1:285:A:PRO:HG3	1:288:A:MET:H	5	0.25
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	1	0.25
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	1	0.25
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD21	2	0.25
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD22	2	0.25
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD23	2	0.25
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD21	2	0.25
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD22	2	0.25
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD23	2	0.25
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD21	2	0.25
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD22	2	0.25
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD23	2	0.25
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	10	0.25
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	10	0.25
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	19	0.25
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	20	0.25
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	14	0.25
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	14	0.25
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	13	0.25
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	13	0.25
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	5	0.25
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	5	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	5	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	5	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	5	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	5	0.25
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	6	0.25
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	6	0.25
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	6	0.25
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	6	0.25
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	13	0.25
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	13	0.25
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	13	0.25
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	13	0.25
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	20	0.25
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	18	0.25
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	18	0.25
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	18	0.25
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD21	9	0.25
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD22	9	0.25
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD21	9	0.25
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD22	9	0.25
(1,135)	1:237:A:ASN:HD21	1:240:A:GLU:H	20	0.25
(1,135)	1:237:A:ASN:HD22	1:240:A:GLU:H	20	0.25
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	11	0.25
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	11	0.25
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	16	0.25
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	20	0.25
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	20	0.25
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	6	0.25
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	6	0.25
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	6	0.25
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	6	0.25
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	9	0.25
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	13	0.25
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	18	0.25
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	14	0.24
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	14	0.24
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	14	0.24
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	9	0.24
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	12	0.24
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	12	0.24
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	12	0.24
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	12	0.24
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	12	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	4	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	4	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	4	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	4	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	4	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	4	0.24
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	4	0.24
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	4	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	20	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	20	0.24
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	20	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	20	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	20	0.24
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	20	0.24
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	20	0.24
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	20	0.24
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	20	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	17	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	17	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	17	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	17	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	17	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	17	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	17	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	17	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	17	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	19	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	19	0.24
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	19	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	19	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	19	0.24
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	19	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	19	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	19	0.24
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	19	0.24
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	20	0.24
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	5	0.24
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	5	0.24
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	5	0.24
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	5	0.24
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	11	0.24
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB2	2	0.24
(1,3466)	1:462:A:ASP:H	1:465:A:ASP:HB3	2	0.24
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	5	0.24
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	6	0.24
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	17	0.24
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	19	0.24
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	20	0.24
(1,3281)	1:441:A:ALA:HB1	1:460:A:LEU:H	10	0.24
(1,3281)	1:441:A:ALA:HB2	1:460:A:LEU:H	10	0.24
(1,3281)	1:441:A:ALA:HB3	1:460:A:LEU:H	10	0.24
(1,3273)	1:440:A:ALA:HA	1:443:A:SER:H	6	0.24
(1,3264)	1:439:A:ALA:HA	1:442:A:LYS:HB2	6	0.24
(1,3264)	1:439:A:ALA:HA	1:442:A:LYS:HB3	6	0.24
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	18	0.24
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	19	0.24
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	19	0.24
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	19	0.24
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	7	0.24
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	10	0.24
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	5	0.24
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	5	0.24
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	5	0.24
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	5	0.24
(1,3153)	1:431:A:TYR:HD1	1:456:A:GLU:H	3	0.24
(1,3153)	1:431:A:TYR:HD2	1:456:A:GLU:H	3	0.24
(1,3143)	1:431:A:TYR:H	1:458:A:LEU:H	15	0.24
(1,3139)	1:431:A:TYR:HA	1:481:A:GLN:H	10	0.24
(1,3126)	1:430:A:ILE:HD11	1:475:A:PHE:H	1	0.24
(1,3126)	1:430:A:ILE:HD12	1:475:A:PHE:H	1	0.24
(1,3126)	1:430:A:ILE:HD13	1:475:A:PHE:H	1	0.24
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	15	0.24
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	15	0.24
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	15	0.24
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	15	0.24
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	2	0.24
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	2	0.24
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	6	0.24
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	6	0.24
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	11	0.24
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	11	0.24
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG2	17	0.24
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG3	17	0.24
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG2	17	0.24
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG3	17	0.24
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG2	17	0.24
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG3	17	0.24
(1,3031)	1:423:A:MET:HE1	1:428:A:GLU:HA	6	0.24
(1,3031)	1:423:A:MET:HE2	1:428:A:GLU:HA	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3031)	1:423:A:MET:HE3	1:428:A:GLU:HA	6	0.24
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	7	0.24
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	7	0.24
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	7	0.24
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	7	0.24
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	7	0.24
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	7	0.24
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	13	0.24
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	13	0.24
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	13	0.24
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	13	0.24
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	13	0.24
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	13	0.24
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	13	0.24
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	13	0.24
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	13	0.24
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	13	0.24
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG11	2	0.24
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG12	2	0.24
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG13	2	0.24
(1,2714)	1:402:A:PHE:HA	1:412:A:GLN:HA	20	0.24
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	4	0.24
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	10	0.24
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	4	0.24
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	14	0.24
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	14	0.24
(1,2594)	1:394:A:GLU:H	1:396:A:ILE:HB	20	0.24
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	7	0.24
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	7	0.24
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	7	0.24
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	7	0.24
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	7	0.24
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	7	0.24
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	7	0.24
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	7	0.24
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	7	0.24
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD11	16	0.24
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD12	16	0.24
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD13	16	0.24
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	18	0.24
(1,2422)	1:383:A:LYS:HD2	1:465:A:ASP:H	18	0.24
(1,2422)	1:383:A:LYS:HD3	1:465:A:ASP:H	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB2	15	0.24
(1,2372)	1:380:A:LEU:HD21	1:462:A:ASP:HB3	15	0.24
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB2	15	0.24
(1,2372)	1:380:A:LEU:HD22	1:462:A:ASP:HB3	15	0.24
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB2	15	0.24
(1,2372)	1:380:A:LEU:HD23	1:462:A:ASP:HB3	15	0.24
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	9	0.24
(1,2300)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	9	0.24
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	7	0.24
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	18	0.24
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	18	0.24
(1,2229)	1:372:A:GLN:HE21	1:376:A:GLN:H	3	0.24
(1,2229)	1:372:A:GLN:HE22	1:376:A:GLN:H	3	0.24
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	20	0.24
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	20	0.24
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	12	0.24
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	11	0.24
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	18	0.24
(1,1781)	1:339:A:LEU:HD21	1:345:A:THR:H	13	0.24
(1,1781)	1:339:A:LEU:HD22	1:345:A:THR:H	13	0.24
(1,1781)	1:339:A:LEU:HD23	1:345:A:THR:H	13	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	4	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	4	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	4	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	9	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	9	0.24
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	9	0.24
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	8	0.24
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	6	0.24
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	6	0.24
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	6	0.24
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	6	0.24
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD2	3	0.24
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD3	3	0.24
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	4	0.24
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	4	0.24
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	8	0.24
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	8	0.24
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	7	0.24
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	1	0.24
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	1	0.24
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	10	0.24
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	10	0.24
(1,1352)	1:305:A:PHE:HE1	1:307:A:MET:HA	2	0.24
(1,1352)	1:305:A:PHE:HE2	1:307:A:MET:HA	2	0.24
(1,1348)	1:305:A:PHE:HZ	1:308:A:ASP:HA	10	0.24
(1,1348)	1:305:A:PHE:HZ	1:308:A:ASP:HA	19	0.24
(1,1323)	1:302:A:GLN:H	1:327:A:SER:H	13	0.24
(1,1320)	1:302:A:GLN:HA	1:328:A:SER:HA	10	0.24
(1,1254)	1:300:A:TYR:HA	1:306:A:ILE:HB	7	0.24
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	11	0.24
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	11	0.24
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	11	0.24
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	11	0.24
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	11	0.24
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	11	0.24
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	11	0.24
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	11	0.24
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	11	0.24
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	1	0.24
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	1	0.24
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	1	0.24
(1,1052)	1:293:A:HIS:HB2	1:295:A:HIS:H	2	0.24
(1,1052)	1:293:A:HIS:HB3	1:295:A:HIS:H	2	0.24
(1,1023)	1:289:A:TRP:HH2	1:381:A:VAL:HA	10	0.24
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	17	0.24
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	17	0.24
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	19	0.24
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	19	0.24
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	19	0.24
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	19	0.24
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	19	0.24
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	19	0.24
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	15	0.24
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	15	0.24
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	15	0.24
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	4	0.24
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	4	0.24
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	11	0.24
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	11	0.24
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB2	6	0.24
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB3	6	0.24
(1,672)	1:270:A:GLY:H	1:273:A:GLU:H	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	15	0.24
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	15	0.24
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	15	0.24
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	15	0.24
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	2	0.24
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	2	0.24
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	3	0.24
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	5	0.24
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	5	0.24
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	5	0.24
(1,423)	1:254:A:ALA:HA	1:323:A:GLY:H	18	0.24
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	15	0.24
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	15	0.24
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	15	0.24
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	15	0.24
(1,371)	1:251:A:LYS:HE2	1:259:A:ASP:HA	16	0.24
(1,371)	1:251:A:LYS:HE3	1:259:A:ASP:HA	16	0.24
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	8	0.24
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	19	0.24
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	8	0.24
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	20	0.24
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	20	0.24
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	5	0.24
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	5	0.24
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	18	0.24
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	18	0.24
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	18	0.24
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	18	0.24
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	1	0.23
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	11	0.23
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	16	0.23
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	19	0.23
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	13	0.23
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	15	0.23
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	15	0.23
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	15	0.23
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	5	0.23
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	5	0.23
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	5	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	5	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	5	0.23
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	5	0.23
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	5	0.23
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	5	0.23
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	5	0.23
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	5	0.23
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	20	0.23
(1,3582)	1:474:A:GLU:H	1:480:A:PHE:H	20	0.23
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	4	0.23
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	4	0.23
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	15	0.23
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	18	0.23
(1,3348)	1:447:A:LEU:HA	1:451:A:ARG:H	14	0.23
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	17	0.23
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	17	0.23
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	17	0.23
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	3	0.23
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	3	0.23
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	3	0.23
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG2	17	0.23
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG3	17	0.23
(1,3263)	1:439:A:ALA:HA	1:442:A:LYS:H	6	0.23
(1,3222)	1:436:A:ASP:H	1:441:A:ALA:H	15	0.23
(1,3220)	1:436:A:ASP:HA	1:463:A:ARG:HA	5	0.23
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	3	0.23
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	18	0.23
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	18	0.23
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	18	0.23
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG2	2	0.23
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG3	2	0.23
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG2	2	0.23
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG3	2	0.23
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG2	7	0.23
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG3	7	0.23
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB2	12	0.23
(1,3033)	1:423:A:MET:HE1	1:427:A:GLN:HB3	12	0.23
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB2	12	0.23
(1,3033)	1:423:A:MET:HE2	1:427:A:GLN:HB3	12	0.23
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB2	12	0.23
(1,3033)	1:423:A:MET:HE3	1:427:A:GLN:HB3	12	0.23
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	12	0.23
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	12	0.23
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB2	5	0.23
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB3	5	0.23
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	10	0.23
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	10	0.23
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	18	0.23
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	18	0.23
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG21	9	0.23
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG22	9	0.23
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG23	9	0.23
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG21	9	0.23
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG22	9	0.23
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG23	9	0.23
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	4	0.23
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	4	0.23
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	14	0.23
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	14	0.23
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	5	0.23
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	5	0.23
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	5	0.23
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	12	0.23
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	12	0.23
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	12	0.23
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	11	0.23
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	11	0.23
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	11	0.23
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	11	0.23
(1,2681)	1:401:A:ARG:HD2	1:414:A:VAL:HA	7	0.23
(1,2681)	1:401:A:ARG:HD3	1:414:A:VAL:HA	7	0.23
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD2	11	0.23
(1,2603)	1:395:A:ALA:HA	1:398:A:LYS:HD3	11	0.23
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	12	0.23
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	16	0.23
(1,2569)	1:393:A:GLN:HE21	1:471:A:TYR:HA	10	0.23
(1,2569)	1:393:A:GLN:HE22	1:471:A:TYR:HA	10	0.23
(1,2563)	1:393:A:GLN:HE21	1:474:A:GLU:H	19	0.23
(1,2563)	1:393:A:GLN:HE22	1:474:A:GLU:H	19	0.23
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	15	0.23
(1,2544)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	15	0.23
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	15	0.23
(1,2544)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	15	0.23
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	19	0.23
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	19	0.23
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	11	0.23
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB2	19	0.23
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB3	19	0.23
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB2	19	0.23
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB3	19	0.23
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD2	18	0.23
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD3	18	0.23
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	8	0.23
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	8	0.23
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	16	0.23
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	11	0.23
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	11	0.23
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	11	0.23
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	11	0.23
(1,2141)	1:365:A:LYS:HA	1:368:A:ALA:HA	18	0.23
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	10	0.23
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	10	0.23
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	10	0.23
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	10	0.23
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	12	0.23
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	12	0.23
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	12	0.23
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	12	0.23
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	14	0.23
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	10	0.23
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	6	0.23
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	13	0.23
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	13	0.23
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	14	0.23
(1,1860)	1:346:A:ARG:HA	1:349:A:ARG:HB2	13	0.23
(1,1860)	1:346:A:ARG:HA	1:349:A:ARG:HB3	13	0.23
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	6	0.23
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	6	0.23
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD11	18	0.23
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD12	18	0.23
(1,1724)	1:334:A:VAL:HA	1:338:A:ILE:HD13	18	0.23
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	11	0.23
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	11	0.23
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	8	0.23
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	8	0.23
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	2	0.23
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	2	0.23
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	2	0.23
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	8	0.23
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	8	0.23
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	10	0.23
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	10	0.23
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	10	0.23
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	16	0.23
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	16	0.23
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	19	0.23
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	19	0.23
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	13	0.23
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	13	0.23
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	13	0.23
(1,1352)	1:305:A:PHE:HE1	1:307:A:MET:HA	18	0.23
(1,1352)	1:305:A:PHE:HE2	1:307:A:MET:HA	18	0.23
(1,1297)	1:301:A:VAL:H	1:306:A:ILE:HB	11	0.23
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	20	0.23
(1,1129)	1:297:A:LEU:H	1:311:A:GLU:HA	6	0.23
(1,1121)	1:297:A:LEU:HD11	1:314:A:MET:HA	1	0.23
(1,1121)	1:297:A:LEU:HD12	1:314:A:MET:HA	1	0.23
(1,1121)	1:297:A:LEU:HD13	1:314:A:MET:HA	1	0.23
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	12	0.23
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	13	0.23
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	2	0.23
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	2	0.23
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	17	0.23
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	4	0.23
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	4	0.23
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	20	0.23
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	20	0.23
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	6	0.23
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	6	0.23
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	6	0.23
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	6	0.23
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	6	0.23
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	6	0.23
(1,945)	1:284:A:ALA:HA	1:320:A:PHE:HB2	7	0.23
(1,945)	1:284:A:ALA:HA	1:320:A:PHE:HB3	7	0.23
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	7	0.23
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	14	0.23
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	18	0.23
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	17	0.23
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	17	0.23
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	15	0.23
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	15	0.23
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	15	0.23
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	6	0.23
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	8	0.23
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	17	0.23
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	17	0.23
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	9	0.23
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	9	0.23
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	9	0.23
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	9	0.23
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	20	0.23
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	20	0.23
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	20	0.23
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	20	0.23
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	18	0.23
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	2	0.23
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	13	0.23
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	16	0.23
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	15	0.23
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	5	0.23
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	17	0.23
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	17	0.23
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	16	0.23
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	9	0.23
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	14	0.23
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	14	0.23
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	14	0.23
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	18	0.23
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	18	0.23
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	1	0.23
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	5	0.23
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	11	0.23
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	5	0.23
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	4	0.22
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	5	0.22
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	13	0.22
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	13	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	13	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	13	0.22
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	13	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	13	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	13	0.22
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	13	0.22
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	11	0.22
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	11	0.22
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	11	0.22
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	18	0.22
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	18	0.22
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	18	0.22
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	18	0.22
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	4	0.22
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	4	0.22
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	4	0.22
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	4	0.22
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	4	0.22
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	4	0.22
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	4	0.22
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	4	0.22
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	4	0.22
(1,3665)	1:399:A:LEU:HD11	2:630:B:LEU:HD11	3	0.22
(1,3665)	1:399:A:LEU:HD11	2:630:B:LEU:HD12	3	0.22
(1,3665)	1:399:A:LEU:HD11	2:630:B:LEU:HD13	3	0.22
(1,3665)	1:399:A:LEU:HD12	2:630:B:LEU:HD11	3	0.22
(1,3665)	1:399:A:LEU:HD12	2:630:B:LEU:HD12	3	0.22
(1,3665)	1:399:A:LEU:HD12	2:630:B:LEU:HD13	3	0.22
(1,3665)	1:399:A:LEU:HD13	2:630:B:LEU:HD11	3	0.22
(1,3665)	1:399:A:LEU:HD13	2:630:B:LEU:HD12	3	0.22
(1,3665)	1:399:A:LEU:HD13	2:630:B:LEU:HD13	3	0.22
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	10	0.22
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	10	0.22
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	10	0.22
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	10	0.22
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	10	0.22
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	10	0.22
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	10	0.22
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	10	0.22
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	10	0.22
(1,3600)	1:475:A:PHE:H	1:480:A:PHE:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	14	0.22
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	14	0.22
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	14	0.22
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	14	0.22
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	11	0.22
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	11	0.22
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	11	0.22
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	9	0.22
(1,3383)	1:450:A:LEU:HB2	1:456:A:GLU:H	16	0.22
(1,3383)	1:450:A:LEU:HB3	1:456:A:GLU:H	16	0.22
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	4	0.22
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	4	0.22
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	1	0.22
(1,3222)	1:436:A:ASP:H	1:441:A:ALA:H	2	0.22
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	3	0.22
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	9	0.22
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	9	0.22
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	9	0.22
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG2	1	0.22
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG3	1	0.22
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	20	0.22
(1,3081)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	12	0.22
(1,3081)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	12	0.22
(1,3081)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	12	0.22
(1,3081)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	12	0.22
(1,3041)	1:424:A:LYS:H	1:455:A:ILE:HA	11	0.22
(1,3031)	1:423:A:MET:HE1	1:428:A:GLU:HA	19	0.22
(1,3031)	1:423:A:MET:HE2	1:428:A:GLU:HA	19	0.22
(1,3031)	1:423:A:MET:HE3	1:428:A:GLU:HA	19	0.22
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	1	0.22
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	1	0.22
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	1	0.22
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	1	0.22
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	1	0.22
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	1	0.22
(1,3013)	1:422:A:ARG:HD2	1:456:A:GLU:HB2	16	0.22
(1,3013)	1:422:A:ARG:HD2	1:456:A:GLU:HB3	16	0.22
(1,3013)	1:422:A:ARG:HD3	1:456:A:GLU:HB2	16	0.22
(1,3013)	1:422:A:ARG:HD3	1:456:A:GLU:HB3	16	0.22
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD2	4	0.22
(1,2828)	1:407:A:THR:HB	1:409:A:SER:H	9	0.22
(1,2822)	1:406:A:HIS:HB2	1:414:A:VAL:HB	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2822)	1:406:A:HIS:HB3	1:414:A:VAL:HB	17	0.22
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	16	0.22
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	16	0.22
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	16	0.22
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	20	0.22
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	20	0.22
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	20	0.22
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	18	0.22
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	14	0.22
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	14	0.22
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	14	0.22
(1,2725)	1:403:A:ALA:H	1:459:A:LEU:H	7	0.22
(1,2572)	1:393:A:GLN:HG2	1:397:A:ALA:H	16	0.22
(1,2572)	1:393:A:GLN:HG3	1:397:A:ALA:H	16	0.22
(1,2565)	1:393:A:GLN:HE21	1:473:A:THR:H	15	0.22
(1,2565)	1:393:A:GLN:HE22	1:473:A:THR:H	15	0.22
(1,2511)	1:387:A:ALA:HA	1:471:A:TYR:HE1	19	0.22
(1,2511)	1:387:A:ALA:HA	1:471:A:TYR:HE2	19	0.22
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	17	0.22
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	5	0.22
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	5	0.22
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	15	0.22
(1,2298)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	15	0.22
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	17	0.22
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE21	5	0.22
(1,2282)	1:375:A:TRP:HE1	1:412:A:GLN:HE22	5	0.22
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	19	0.22
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	2	0.22
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	2	0.22
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	2	0.22
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	2	0.22
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	16	0.22
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	16	0.22
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	2	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	4	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	4	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	4	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	9	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	9	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	9	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	10	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	10	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	12	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	12	0.22
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	12	0.22
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	9	0.22
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	9	0.22
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	5	0.22
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	4	0.22
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	4	0.22
(1,1815)	1:343:A:THR:HA	1:347:A:ASN:H	6	0.22
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	3	0.22
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	3	0.22
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	6	0.22
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	6	0.22
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	7	0.22
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	7	0.22
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	12	0.22
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	12	0.22
(1,1351)	1:305:A:PHE:HZ	1:307:A:MET:HA	2	0.22
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	15	0.22
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	15	0.22
(1,1155)	1:298:A:LYS:H	1:323:A:GLY:H	9	0.22
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	18	0.22
(1,1089)	1:296:A:GLY:H	1:311:A:GLU:HA	7	0.22
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	5	0.22
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	5	0.22
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	19	0.22
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	19	0.22
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	13	0.22
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	8	0.22
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	8	0.22
(1,936)	1:284:A:ALA:HA	1:378:A:PHE:HZ	14	0.22
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	16	0.22
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	16	0.22
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	16	0.22
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	15	0.22
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	15	0.22
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	15	0.22
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	15	0.22
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	15	0.22
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	15	0.22
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	19	0.22
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB2	16	0.22
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB3	16	0.22
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB2	1	0.22
(1,674)	1:270:A:GLY:H	1:273:A:GLU:HB3	1	0.22
(1,672)	1:270:A:GLY:H	1:273:A:GLU:H	20	0.22
(1,666)	1:269:A:GLU:H	1:273:A:GLU:HA	7	0.22
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	14	0.22
(1,475)	1:260:A:PRO:HA	1:280:A:ILE:H	11	0.22
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	20	0.22
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	12	0.22
(1,425)	1:254:A:ALA:HB1	1:322:A:ARG:HB2	2	0.22
(1,425)	1:254:A:ALA:HB1	1:322:A:ARG:HB3	2	0.22
(1,425)	1:254:A:ALA:HB2	1:322:A:ARG:HB2	2	0.22
(1,425)	1:254:A:ALA:HB2	1:322:A:ARG:HB3	2	0.22
(1,425)	1:254:A:ALA:HB3	1:322:A:ARG:HB2	2	0.22
(1,425)	1:254:A:ALA:HB3	1:322:A:ARG:HB3	2	0.22
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	12	0.22
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	12	0.22
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	16	0.22
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	7	0.22
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	11	0.22
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD2	7	0.22
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD3	7	0.22
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD2	7	0.22
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD3	7	0.22
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	15	0.22
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	17	0.22
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	18	0.22
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	2	0.22
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	2	0.22
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	4	0.22
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	7	0.22
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	14	0.22
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	13	0.21
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	17	0.21
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	7	0.21
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	7	0.21
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	7	0.21
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	7	0.21
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	7	0.21
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	7	0.21
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	7	0.21
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	7	0.21
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	2	0.21
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	2	0.21
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	2	0.21
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	2	0.21
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	2	0.21
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	2	0.21
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	2	0.21
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	2	0.21
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	2	0.21
(1,3619)	1:476:A:ASP:HB2	1:478:A:LYS:HD2	20	0.21
(1,3619)	1:476:A:ASP:HB2	1:478:A:LYS:HD3	20	0.21
(1,3619)	1:476:A:ASP:HB3	1:478:A:LYS:HD2	20	0.21
(1,3619)	1:476:A:ASP:HB3	1:478:A:LYS:HD3	20	0.21
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	16	0.21
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	13	0.21
(1,3582)	1:474:A:GLU:H	1:480:A:PHE:H	13	0.21
(1,3577)	1:473:A:THR:HA	1:479:A:PRO:HA	13	0.21
(1,3539)	1:469:A:MET:HE1	1:473:A:THR:H	5	0.21
(1,3539)	1:469:A:MET:HE2	1:473:A:THR:H	5	0.21
(1,3539)	1:469:A:MET:HE3	1:473:A:THR:H	5	0.21
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	10	0.21
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	10	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	10	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	10	0.21
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	13	0.21
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	13	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	13	0.21
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	13	0.21
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	11	0.21
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	11	0.21
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	11	0.21
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	11	0.21
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	11	0.21
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	11	0.21
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	9	0.21
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	3	0.21
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	12	0.21
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	12	0.21
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	12	0.21
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	16	0.21
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	16	0.21
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	11	0.21
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	15	0.21
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	19	0.21
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	20	0.21
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	20	0.21
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	20	0.21
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	15	0.21
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	9	0.21
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	11	0.21
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	12	0.21
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	16	0.21
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	20	0.21
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	20	0.21
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	20	0.21
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	20	0.21
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG2	3	0.21
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG3	3	0.21
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG2	6	0.21
(1,3084)	1:428:A:GLU:HA	1:478:A:LYS:HG3	6	0.21
(1,3043)	1:424:A:LYS:HG2	1:455:A:ILE:HA	4	0.21
(1,3043)	1:424:A:LYS:HG3	1:455:A:ILE:HA	4	0.21
(1,2945)	1:417:A:GLU:HB2	1:418:A:ASP:H	19	0.21
(1,2945)	1:417:A:GLU:HB3	1:418:A:ASP:H	19	0.21
(1,2932)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	7	0.21
(1,2932)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	7	0.21
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	16	0.21
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	16	0.21
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD11	1	0.21
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD12	1	0.21
(1,2857)	1:410:A:SER:HA	1:459:A:LEU:HD13	1	0.21
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	13	0.21
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	13	0.21
(1,2714)	1:402:A:PHE:HA	1:412:A:GLN:HA	8	0.21
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	11	0.21
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	7	0.21
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	7	0.21
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	7	0.21
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	7	0.21
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2602)	1:395:A:ALA:HA	1:398:A:LYS:HB3	7	0.21
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	4	0.21
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	4	0.21
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	4	0.21
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	4	0.21
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	6	0.21
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	15	0.21
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	4	0.21
(1,2379)	1:380:A:LEU:H	1:382:A:LEU:H	8	0.21
(1,2357)	1:379:A:GLY:H	1:382:A:LEU:H	12	0.21
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	8	0.21
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	6	0.21
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	18	0.21
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	1	0.21
(1,2009)	1:358:A:GLN:HA	1:361:A:GLU:H	6	0.21
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB2	13	0.21
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB3	13	0.21
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	18	0.21
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	18	0.21
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	20	0.21
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB2	16	0.21
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB3	16	0.21
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB2	16	0.21
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB3	16	0.21
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	11	0.21
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	11	0.21
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	6	0.21
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	10	0.21
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	10	0.21
(1,1421)	1:312:A:GLN:HE21	1:340:A:GLN:HA	15	0.21
(1,1421)	1:312:A:GLN:HE22	1:340:A:GLN:HA	15	0.21
(1,1323)	1:302:A:GLN:H	1:327:A:SER:H	6	0.21
(1,1297)	1:301:A:VAL:H	1:306:A:ILE:HB	7	0.21
(1,1214)	1:299:A:LEU:H	1:307:A:MET:H	9	0.21
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	20	0.21
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	6	0.21
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	6	0.21
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	1	0.21
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	1	0.21
(1,1023)	1:289:A:TRP:HH2	1:381:A:VAL:HA	13	0.21
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	18	0.21
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	20	0.21
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	14	0.21
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	14	0.21
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	14	0.21
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	12	0.21
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	2	0.21
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	2	0.21
(1,699)	1:273:A:GLU:H	1:329:A:ASP:H	16	0.21
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	5	0.21
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	13	0.21
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	13	0.21
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	13	0.21
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	15	0.21
(1,575)	1:264:A:SER:HB2	1:356:A:VAL:HA	2	0.21
(1,575)	1:264:A:SER:HB3	1:356:A:VAL:HA	2	0.21
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	19	0.21
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	8	0.21
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	6	0.21
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	8	0.21
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	17	0.21
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	18	0.21
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	2	0.21
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	19	0.21
(1,370)	1:251:A:LYS:HE2	1:259:A:ASP:H	16	0.21
(1,370)	1:251:A:LYS:HE3	1:259:A:ASP:H	16	0.21
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	16	0.21
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	16	0.21
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	20	0.21
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	2	0.21
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	2	0.21
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	6	0.21
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	9	0.21
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	12	0.21
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	11	0.21
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	2	0.21
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	5	0.2
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	15	0.2
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	11	0.2
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	11	0.2
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD21	20	0.2
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD22	20	0.2
(1,3678)	1:317:A:TYR:HE1	2:628:B:LEU:HD23	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD21	20	0.2
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD22	20	0.2
(1,3678)	1:317:A:TYR:HE2	2:628:B:LEU:HD23	20	0.2
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	3	0.2
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	3	0.2
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	3	0.2
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	3	0.2
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	3	0.2
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	3	0.2
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	3	0.2
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	3	0.2
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	3	0.2
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	19	0.2
(1,3577)	1:473:A:THR:HA	1:479:A:PRO:HA	15	0.2
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	5	0.2
(1,3553)	1:470:A:ASN:HA	1:472:A:LEU:H	8	0.2
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	16	0.2
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	16	0.2
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	17	0.2
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	17	0.2
(1,3509)	1:466:A:GLU:HA	1:469:A:MET:HB2	8	0.2
(1,3509)	1:466:A:GLU:HA	1:469:A:MET:HB3	8	0.2
(1,3505)	1:465:A:ASP:HB2	1:466:A:GLU:H	19	0.2
(1,3505)	1:465:A:ASP:HB3	1:466:A:GLU:H	19	0.2
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG2	10	0.2
(1,3494)	1:465:A:ASP:HA	1:469:A:MET:HG3	10	0.2
(1,3460)	1:461:A:SER:H	1:465:A:ASP:HB2	2	0.2
(1,3460)	1:461:A:SER:H	1:465:A:ASP:HB3	2	0.2
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	12	0.2
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	12	0.2
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	12	0.2
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB2	1	0.2
(1,3327)	1:445:A:PRO:HA	1:448:A:GLU:HB3	1	0.2
(1,3317)	1:444:A:SER:H	1:447:A:LEU:H	14	0.2
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	17	0.2
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	17	0.2
(1,3210)	1:435:A:ALA:H	1:460:A:LEU:H	7	0.2
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB2	6	0.2
(1,3206)	1:435:A:ALA:H	1:465:A:ASP:HB3	6	0.2
(1,3200)	1:434:A:THR:HA	1:461:A:SER:HA	8	0.2
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	13	0.2
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	14	0.2
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	5	0.2
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	5	0.2
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	5	0.2
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	5	0.2
(1,2945)	1:417:A:GLU:HB2	1:418:A:ASP:H	7	0.2
(1,2945)	1:417:A:GLU:HB3	1:418:A:ASP:H	7	0.2
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	10	0.2
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	10	0.2
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	10	0.2
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	10	0.2
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	10	0.2
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	10	0.2
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	10	0.2
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	10	0.2
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	10	0.2
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	2	0.2
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	2	0.2
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	15	0.2
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	15	0.2
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	15	0.2
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG11	1	0.2
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG12	1	0.2
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG13	1	0.2
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	3	0.2
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	12	0.2
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	12	0.2
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	12	0.2
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	11	0.2
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD2	1	0.2
(1,2588)	1:394:A:GLU:HG2	1:398:A:LYS:HD3	1	0.2
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD2	1	0.2
(1,2588)	1:394:A:GLU:HG3	1:398:A:LYS:HD3	1	0.2
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	9	0.2
(1,2565)	1:393:A:GLN:HE21	1:473:A:THR:H	20	0.2
(1,2565)	1:393:A:GLN:HE22	1:473:A:THR:H	20	0.2
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	18	0.2
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	16	0.2
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD11	11	0.2
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD12	11	0.2
(1,2528)	1:388:A:GLU:H	1:396:A:ILE:HD13	11	0.2
(1,2517)	1:387:A:ALA:H	1:467:A:TRP:HH2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2469)	1:385:A:GLY:HA2	1:389:A:ASP:H	12	0.2
(1,2469)	1:385:A:GLY:HA3	1:389:A:ASP:H	12	0.2
(1,2469)	1:385:A:GLY:HA2	1:389:A:ASP:H	16	0.2
(1,2469)	1:385:A:GLY:HA3	1:389:A:ASP:H	16	0.2
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	7	0.2
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	10	0.2
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	15	0.2
(1,2294)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	6	0.2
(1,2294)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	16	0.2
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	12	0.2
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	12	0.2
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	9	0.2
(1,2141)	1:365:A:LYS:HA	1:368:A:ALA:HA	16	0.2
(1,2141)	1:365:A:LYS:HA	1:368:A:ALA:HA	17	0.2
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	14	0.2
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	14	0.2
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	14	0.2
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	15	0.2
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	15	0.2
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	15	0.2
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	15	0.2
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	15	0.2
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	15	0.2
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	13	0.2
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	13	0.2
(1,1939)	1:353:A:THR:HG21	1:396:A:ILE:HD11	13	0.2
(1,1939)	1:353:A:THR:HG21	1:396:A:ILE:HD12	13	0.2
(1,1939)	1:353:A:THR:HG21	1:396:A:ILE:HD13	13	0.2
(1,1939)	1:353:A:THR:HG22	1:396:A:ILE:HD11	13	0.2
(1,1939)	1:353:A:THR:HG22	1:396:A:ILE:HD12	13	0.2
(1,1939)	1:353:A:THR:HG22	1:396:A:ILE:HD13	13	0.2
(1,1939)	1:353:A:THR:HG23	1:396:A:ILE:HD11	13	0.2
(1,1939)	1:353:A:THR:HG23	1:396:A:ILE:HD12	13	0.2
(1,1939)	1:353:A:THR:HG23	1:396:A:ILE:HD13	13	0.2
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	20	0.2
(1,1853)	1:345:A:THR:HB	1:346:A:ARG:HB2	16	0.2
(1,1853)	1:345:A:THR:HB	1:346:A:ARG:HB3	16	0.2
(1,1732)	1:335:A:SER:H	1:339:A:LEU:H	19	0.2
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	1	0.2
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	3	0.2
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	3	0.2
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	2	0.2
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	13	0.2
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	13	0.2
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	11	0.2
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	11	0.2
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	20	0.2
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	7	0.2
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	7	0.2
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	18	0.2
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	14	0.2
(1,1096)	1:296:A:GLY:H	1:309:A:ASP:HA	3	0.2
(1,1095)	1:296:A:GLY:HA2	1:309:A:ASP:H	20	0.2
(1,1095)	1:296:A:GLY:HA3	1:309:A:ASP:H	20	0.2
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	15	0.2
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	20	0.2
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	17	0.2
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	10	0.2
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	10	0.2
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	10	0.2
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	19	0.2
(1,743)	1:275:A:THR:H	1:326:A:ASP:H	9	0.2
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB2	12	0.2
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB3	12	0.2
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	9	0.2
(1,652)	1:268:A:VAL:H	1:273:A:GLU:HA	7	0.2
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	7	0.2
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	9	0.2
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	9	0.2
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	11	0.2
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	3	0.2
(1,418)	1:253:A:ILE:HD11	1:255:A:HIS:H	6	0.2
(1,418)	1:253:A:ILE:HD12	1:255:A:HIS:H	6	0.2
(1,418)	1:253:A:ILE:HD13	1:255:A:HIS:H	6	0.2
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	2	0.2
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	2	0.2
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	2	0.2
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	2	0.2
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	1	0.2
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	2	0.2
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	15	0.2
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	7	0.2
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:238:A:LYS:HA	1:265:A:HIS:HE1	1	0.2
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	2	0.2
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	2	0.2
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	2	0.2
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	2	0.2
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	7	0.2
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	8	0.2
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	18	0.2
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	7	0.2
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	7	0.2
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	15	0.2
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	9	0.19
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	14	0.19
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	14	0.19
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	13	0.19
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	13	0.19
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	13	0.19
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG11	3	0.19
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG12	3	0.19
(1,3655)	1:483:A:VAL:HG11	2:615:B:VAL:HG13	3	0.19
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG11	3	0.19
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG12	3	0.19
(1,3655)	1:483:A:VAL:HG12	2:615:B:VAL:HG13	3	0.19
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG11	3	0.19
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG12	3	0.19
(1,3655)	1:483:A:VAL:HG13	2:615:B:VAL:HG13	3	0.19
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	12	0.19
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	12	0.19
(1,3599)	1:474:A:GLU:HG2	1:475:A:PHE:H	4	0.19
(1,3599)	1:474:A:GLU:HG3	1:475:A:PHE:H	4	0.19
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	3	0.19
(1,3578)	1:473:A:THR:HB	1:479:A:PRO:HA	13	0.19
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	10	0.19
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	12	0.19
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	12	0.19
(1,3493)	1:465:A:ASP:HA	1:469:A:MET:H	8	0.19
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	3	0.19
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	7	0.19
(1,3485)	1:464:A:ILE:HA	1:467:A:TRP:HE3	18	0.19
(1,3425)	1:455:A:ILE:HB	1:456:A:GLU:H	1	0.19
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	4	0.19
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	15	0.19
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	15	0.19
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG2	11	0.19
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG3	11	0.19
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG2	19	0.19
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG3	19	0.19
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	10	0.19
(1,3181)	1:433:A:ILE:H	1:460:A:LEU:H	18	0.19
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	19	0.19
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	19	0.19
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	1	0.19
(1,3159)	1:432:A:TYR:H	1:482:A:SER:HA	12	0.19
(1,3119)	1:430:A:ILE:HD11	1:479:A:PRO:HA	19	0.19
(1,3119)	1:430:A:ILE:HD12	1:479:A:PRO:HA	19	0.19
(1,3119)	1:430:A:ILE:HD13	1:479:A:PRO:HA	19	0.19
(1,3106)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	14	0.19
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	17	0.19
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	17	0.19
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	17	0.19
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	17	0.19
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD1	13	0.19
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	9	0.19
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	9	0.19
(1,2836)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	7	0.19
(1,2826)	1:406:A:HIS:HB2	1:407:A:THR:H	9	0.19
(1,2826)	1:406:A:HIS:HB3	1:407:A:THR:H	9	0.19
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	15	0.19
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	15	0.19
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	3	0.19
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	3	0.19
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	3	0.19
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	3	0.19
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	3	0.19
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	3	0.19
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	7	0.19
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG11	3	0.19
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG12	3	0.19
(1,2771)	1:404:A:SER:H	1:414:A:VAL:HG13	3	0.19
(1,2758)	1:404:A:SER:HB2	1:458:A:LEU:HA	1	0.19
(1,2758)	1:404:A:SER:HB3	1:458:A:LEU:HA	1	0.19
(1,2725)	1:403:A:ALA:H	1:459:A:LEU:H	2	0.19
(1,2709)	1:402:A:PHE:H	1:414:A:VAL:HB	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	8	0.19
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	19	0.19
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	14	0.19
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	10	0.19
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	5	0.19
(1,2366)	1:380:A:LEU:HB2	1:464:A:ILE:H	3	0.19
(1,2366)	1:380:A:LEU:HB3	1:464:A:ILE:H	3	0.19
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE21	5	0.19
(1,2322)	1:376:A:GLN:HA	1:412:A:GLN:HE22	5	0.19
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	1	0.19
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	1	0.19
(1,2321)	1:376:A:GLN:HE21	1:412:A:GLN:H	3	0.19
(1,2321)	1:376:A:GLN:HE22	1:412:A:GLN:H	3	0.19
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	16	0.19
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE1	20	0.19
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE2	20	0.19
(1,2276)	1:375:A:TRP:HH2	1:468:A:MET:HE3	20	0.19
(1,2264)	1:374:A:PHE:HZ	1:378:A:PHE:HB2	4	0.19
(1,2264)	1:374:A:PHE:HZ	1:378:A:PHE:HB3	4	0.19
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	1	0.19
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	1	0.19
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	20	0.19
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	11	0.19
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	11	0.19
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	11	0.19
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	11	0.19
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	12	0.19
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	12	0.19
(1,2008)	1:358:A:GLN:H	1:361:A:GLU:H	4	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	1	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	1	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	1	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	16	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	16	0.19
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	16	0.19
(1,1880)	1:348:A:LEU:HD11	1:352:A:LEU:H	19	0.19
(1,1880)	1:348:A:LEU:HD12	1:352:A:LEU:H	19	0.19
(1,1880)	1:348:A:LEU:HD13	1:352:A:LEU:H	19	0.19
(1,1758)	1:337:A:GLU:HA	1:341:A:ASP:H	15	0.19
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	3	0.19
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	3	0.19
(1,1644)	1:325:A:ILE:HD11	1:327:A:SER:H	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:325:A:ILE:HD12	1:327:A:SER:H	14	0.19
(1,1644)	1:325:A:ILE:HD13	1:327:A:SER:H	14	0.19
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	6	0.19
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	12	0.19
(1,1533)	1:317:A:TYR:HB2	1:385:A:GLY:H	15	0.19
(1,1533)	1:317:A:TYR:HB3	1:385:A:GLY:H	15	0.19
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB2	12	0.19
(1,1531)	1:317:A:TYR:HB2	1:388:A:GLU:HB3	12	0.19
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB2	12	0.19
(1,1531)	1:317:A:TYR:HB3	1:388:A:GLU:HB3	12	0.19
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	11	0.19
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	11	0.19
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	11	0.19
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	11	0.19
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD2	10	0.19
(1,1504)	1:315:A:PRO:HA	1:349:A:ARG:HD3	10	0.19
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	4	0.19
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	4	0.19
(1,1500)	1:315:A:PRO:HG2	1:353:A:THR:HA	20	0.19
(1,1500)	1:315:A:PRO:HG3	1:353:A:THR:HA	20	0.19
(1,1487)	1:314:A:MET:HG2	1:319:A:ARG:HA	20	0.19
(1,1487)	1:314:A:MET:HG3	1:319:A:ARG:HA	20	0.19
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD11	11	0.19
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD12	11	0.19
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD13	11	0.19
(1,1376)	1:307:A:MET:HB2	1:310:A:ALA:H	3	0.19
(1,1376)	1:307:A:MET:HB3	1:310:A:ALA:H	3	0.19
(1,1368)	1:307:A:MET:HE1	1:337:A:GLU:H	13	0.19
(1,1368)	1:307:A:MET:HE2	1:337:A:GLU:H	13	0.19
(1,1368)	1:307:A:MET:HE3	1:337:A:GLU:H	13	0.19
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	16	0.19
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	16	0.19
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	19	0.19
(1,1129)	1:297:A:LEU:H	1:311:A:GLU:HA	15	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	13	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	13	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	17	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	17	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	20	0.19
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	20	0.19
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	7	0.19
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	11	0.19
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	11	0.19
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	15	0.19
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	7	0.19
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	14	0.19
(1,781)	1:277:A:LEU:H	1:324:A:LEU:H	2	0.19
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	7	0.19
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	7	0.19
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	8	0.19
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	8	0.19
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	14	0.19
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	14	0.19
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	15	0.19
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	15	0.19
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	17	0.19
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	3	0.19
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	17	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	3	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	3	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	3	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	3	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	12	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	12	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	12	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	12	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	14	0.19
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	14	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	14	0.19
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	14	0.19
(1,338)	1:250:A:TYR:HD1	1:280:A:ILE:H	18	0.19
(1,338)	1:250:A:TYR:HD2	1:280:A:ILE:H	18	0.19
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	5	0.19
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	4	0.19
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	6	0.19
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	16	0.19
(1,194)	1:242:A:THR:H	1:245:A:GLU:HB2	5	0.19
(1,194)	1:242:A:THR:H	1:245:A:GLU:HB3	5	0.19
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	1	0.19
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	3	0.19
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	10	0.19
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	12	0.19
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	3	0.18
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	3	0.18
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	10	0.18
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	10	0.18
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	10	0.18
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	16	0.18
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	16	0.18
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	16	0.18
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	16	0.18
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	16	0.18
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	16	0.18
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	16	0.18
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	16	0.18
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	16	0.18
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	15	0.18
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	15	0.18
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	15	0.18
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	18	0.18
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	18	0.18
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	18	0.18
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	18	0.18
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	18	0.18
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	18	0.18
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	18	0.18
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	18	0.18
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	18	0.18
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	14	0.18
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	14	0.18
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	14	0.18
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	14	0.18
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	14	0.18
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	14	0.18
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	14	0.18
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	14	0.18
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	14	0.18
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	19	0.18
(1,3591)	1:474:A:GLU:HG2	1:478:A:LYS:H	4	0.18
(1,3591)	1:474:A:GLU:HG3	1:478:A:LYS:H	4	0.18
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	4	0.18
(1,3582)	1:474:A:GLU:H	1:480:A:PHE:H	7	0.18
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	1	0.18
(1,3525)	1:468:A:MET:HA	1:472:A:LEU:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3514)	1:467:A:TRP:HZ2	1:471:A:TYR:HE1	12	0.18
(1,3514)	1:467:A:TRP:HZ2	1:471:A:TYR:HE2	12	0.18
(1,3366)	1:448:A:GLU:HA	1:450:A:LEU:H	20	0.18
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	9	0.18
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	9	0.18
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	9	0.18
(1,3326)	1:445:A:PRO:HA	1:448:A:GLU:H	10	0.18
(1,3263)	1:439:A:ALA:HA	1:442:A:LYS:H	8	0.18
(1,3226)	1:437:A:SER:H	1:461:A:SER:HA	5	0.18
(1,3222)	1:436:A:ASP:H	1:441:A:ALA:H	9	0.18
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	15	0.18
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	5	0.18
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	4	0.18
(1,3171)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	4	0.18
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	4	0.18
(1,3171)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	4	0.18
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	6	0.18
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	6	0.18
(1,3169)	1:432:A:TYR:HB2	1:458:A:LEU:H	13	0.18
(1,3169)	1:432:A:TYR:HB3	1:458:A:LEU:H	13	0.18
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	7	0.18
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	7	0.18
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	7	0.18
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG2	6	0.18
(1,3099)	1:429:A:LYS:HE2	1:479:A:PRO:HG3	6	0.18
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG2	6	0.18
(1,3099)	1:429:A:LYS:HE3	1:479:A:PRO:HG3	6	0.18
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	10	0.18
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB2	17	0.18
(1,3092)	1:429:A:LYS:HG2	1:481:A:GLN:HB3	17	0.18
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB2	17	0.18
(1,3092)	1:429:A:LYS:HG3	1:481:A:GLN:HB3	17	0.18
(1,3041)	1:424:A:LYS:H	1:455:A:ILE:HA	12	0.18
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE21	2	0.18
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE22	2	0.18
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	2	0.18
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	2	0.18
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	2	0.18
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	2	0.18
(1,2969)	1:419:A:TYR:HE1	1:431:A:TYR:H	11	0.18
(1,2969)	1:419:A:TYR:HE2	1:431:A:TYR:H	11	0.18
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	17	0.18
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	17	0.18
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG21	1	0.18
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG22	1	0.18
(1,2848)	1:409:A:SER:HB2	1:413:A:THR:HG23	1	0.18
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG21	1	0.18
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG22	1	0.18
(1,2848)	1:409:A:SER:HB3	1:413:A:THR:HG23	1	0.18
(1,2809)	1:405:A:THR:HG21	1:408:A:ASP:HA	11	0.18
(1,2809)	1:405:A:THR:HG22	1:408:A:ASP:HA	11	0.18
(1,2809)	1:405:A:THR:HG23	1:408:A:ASP:HA	11	0.18
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	13	0.18
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	14	0.18
(1,2776)	1:404:A:SER:H	1:407:A:THR:HB	13	0.18
(1,2710)	1:402:A:PHE:H	1:414:A:VAL:HG11	14	0.18
(1,2710)	1:402:A:PHE:H	1:414:A:VAL:HG12	14	0.18
(1,2710)	1:402:A:PHE:H	1:414:A:VAL:HG13	14	0.18
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	10	0.18
(1,2556)	1:392:A:ASN:HA	1:396:A:ILE:H	7	0.18
(1,2508)	1:387:A:ALA:HA	1:471:A:TYR:HB2	16	0.18
(1,2508)	1:387:A:ALA:HA	1:471:A:TYR:HB3	16	0.18
(1,2469)	1:385:A:GLY:HA2	1:389:A:ASP:H	14	0.18
(1,2469)	1:385:A:GLY:HA3	1:389:A:ASP:H	14	0.18
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	1	0.18
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	7	0.18
(1,2339)	1:378:A:PHE:HA	1:382:A:LEU:H	16	0.18
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	1	0.18
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	5	0.18
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	5	0.18
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	20	0.18
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	20	0.18
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	2	0.18
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	2	0.18
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	2	0.18
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	2	0.18
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	2	0.18
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	2	0.18
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	8	0.18
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	11	0.18
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	8	0.18
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	8	0.18
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	7	0.18
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	7	0.18
(1,1797)	1:340:A:GLN:HA	1:342:A:SER:H	3	0.18
(1,1797)	1:340:A:GLN:HA	1:342:A:SER:H	9	0.18
(1,1762)	1:337:A:GLU:HA	1:340:A:GLN:H	16	0.18
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD11	7	0.18
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD12	7	0.18
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD13	7	0.18
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	14	0.18
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	4	0.18
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	4	0.18
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	8	0.18
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	8	0.18
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	3	0.18
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	3	0.18
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	20	0.18
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	20	0.18
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	20	0.18
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	20	0.18
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	4	0.18
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	4	0.18
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	4	0.18
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	2	0.18
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	3	0.18
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	4	0.18
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	14	0.18
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	14	0.18
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	14	0.18
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	14	0.18
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	14	0.18
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	14	0.18
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	14	0.18
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	14	0.18
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	14	0.18
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	17	0.18
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	17	0.18
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	17	0.18
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	1	0.18
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	4	0.18
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	14	0.18
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	15	0.18
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	16	0.18
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	16	0.18
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	17	0.18
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	17	0.18
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	10	0.18
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	10	0.18
(1,676)	1:270:A:GLY:HA2	1:272:A:GLN:H	9	0.18
(1,676)	1:270:A:GLY:HA3	1:272:A:GLN:H	9	0.18
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	1	0.18
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	16	0.18
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	10	0.18
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	10	0.18
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	16	0.18
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	1	0.18
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	13	0.18
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	13	0.18
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	12	0.18
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE2	15	0.18
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE3	15	0.18
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	6	0.18
(1,268)	1:247:A:LYS:HE2	1:263:A:TRP:HZ3	1	0.18
(1,268)	1:247:A:LYS:HE3	1:263:A:TRP:HZ3	1	0.18
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	11	0.18
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	14	0.18
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	5	0.18
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	15	0.18
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	8	0.18
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	8	0.18
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	13	0.18
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	13	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	7	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	7	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	8	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	8	0.18
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	14	0.18
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	12	0.17
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	12	0.17
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	12	0.17
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	18	0.17
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	18	0.17
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	18	0.17
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	12	0.17
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	12	0.17
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	12	0.17
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	12	0.17
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	12	0.17
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	12	0.17
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	12	0.17
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	12	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	1	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	1	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	1	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	1	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	1	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	1	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	1	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	1	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	1	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	5	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	5	0.17
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	5	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	5	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	5	0.17
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	5	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	5	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	5	0.17
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	5	0.17
(1,3639)	1:481:A:GLN:HE21	1:482:A:SER:H	10	0.17
(1,3639)	1:481:A:GLN:HE22	1:482:A:SER:H	10	0.17
(1,3607)	1:475:A:PHE:H	1:478:A:LYS:H	10	0.17
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	14	0.17
(1,3528)	1:468:A:MET:HA	1:471:A:TYR:H	14	0.17
(1,3497)	1:465:A:ASP:HA	1:468:A:MET:H	20	0.17
(1,3482)	1:464:A:ILE:HD11	1:468:A:MET:H	19	0.17
(1,3482)	1:464:A:ILE:HD12	1:468:A:MET:H	19	0.17
(1,3482)	1:464:A:ILE:HD13	1:468:A:MET:H	19	0.17
(1,3481)	1:464:A:ILE:HA	1:468:A:MET:H	8	0.17
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE1	6	0.17
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE2	6	0.17
(1,3443)	1:458:A:LEU:HD11	1:469:A:MET:HE3	6	0.17
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE1	6	0.17
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE2	6	0.17
(1,3443)	1:458:A:LEU:HD12	1:469:A:MET:HE3	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE1	6	0.17
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE2	6	0.17
(1,3443)	1:458:A:LEU:HD13	1:469:A:MET:HE3	6	0.17
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	14	0.17
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	15	0.17
(1,3349)	1:447:A:LEU:HB2	1:451:A:ARG:H	10	0.17
(1,3349)	1:447:A:LEU:HB3	1:451:A:ARG:H	10	0.17
(1,3221)	1:436:A:ASP:HA	1:461:A:SER:HA	14	0.17
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	2	0.17
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	2	0.17
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	2	0.17
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	14	0.17
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	14	0.17
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	14	0.17
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	14	0.17
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB2	20	0.17
(1,3102)	1:429:A:LYS:HA	1:478:A:LYS:HB3	20	0.17
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	4	0.17
(1,3062)	1:426:A:GLY:HA2	1:428:A:GLU:HA	4	0.17
(1,3062)	1:426:A:GLY:HA3	1:428:A:GLU:HA	4	0.17
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	5	0.17
(1,3015)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	5	0.17
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	5	0.17
(1,3015)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	5	0.17
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	5	0.17
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	9	0.17
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	9	0.17
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	9	0.17
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	9	0.17
(1,2817)	1:406:A:HIS:H	1:456:A:GLU:HA	14	0.17
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	19	0.17
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	19	0.17
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	19	0.17
(1,2756)	1:404:A:SER:HB2	1:458:A:LEU:H	18	0.17
(1,2756)	1:404:A:SER:HB3	1:458:A:LEU:H	18	0.17
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	8	0.17
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	8	0.17
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	8	0.17
(1,2714)	1:402:A:PHE:HA	1:412:A:GLN:HA	18	0.17
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	17	0.17
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	3	0.17
(1,2587)	1:394:A:GLU:HG2	1:398:A:LYS:H	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2587)	1:394:A:GLU:HG3	1:398:A:LYS:H	13	0.17
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	1	0.17
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	4	0.17
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	15	0.17
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD11	1	0.17
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD12	1	0.17
(1,2533)	1:389:A:ASP:H	1:396:A:ILE:HD13	1	0.17
(1,2526)	1:388:A:GLU:H	1:467:A:TRP:HH2	16	0.17
(1,2428)	1:383:A:LYS:HB2	1:464:A:ILE:HD11	17	0.17
(1,2428)	1:383:A:LYS:HB2	1:464:A:ILE:HD12	17	0.17
(1,2428)	1:383:A:LYS:HB2	1:464:A:ILE:HD13	17	0.17
(1,2428)	1:383:A:LYS:HB3	1:464:A:ILE:HD11	17	0.17
(1,2428)	1:383:A:LYS:HB3	1:464:A:ILE:HD12	17	0.17
(1,2428)	1:383:A:LYS:HB3	1:464:A:ILE:HD13	17	0.17
(1,2387)	1:381:A:VAL:HA	1:385:A:GLY:H	12	0.17
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	6	0.17
(1,2258)	1:374:A:PHE:HZ	1:382:A:LEU:H	3	0.17
(1,2230)	1:372:A:GLN:HE21	1:376:A:GLN:HE21	18	0.17
(1,2230)	1:372:A:GLN:HE21	1:376:A:GLN:HE22	18	0.17
(1,2230)	1:372:A:GLN:HE22	1:376:A:GLN:HE21	18	0.17
(1,2230)	1:372:A:GLN:HE22	1:376:A:GLN:HE22	18	0.17
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	20	0.17
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	1	0.17
(1,2138)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	1	0.17
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	1	0.17
(1,2138)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	1	0.17
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	4	0.17
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	4	0.17
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	14	0.17
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	4	0.17
(1,1891)	1:349:A:ARG:HA	1:353:A:THR:H	4	0.17
(1,1852)	1:345:A:THR:HB	1:346:A:ARG:H	6	0.17
(1,1828)	1:344:A:VAL:HA	1:348:A:LEU:H	8	0.17
(1,1786)	1:339:A:LEU:HA	1:342:A:SER:H	18	0.17
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	3	0.17
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	3	0.17
(1,1715)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	3	0.17
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	3	0.17
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	3	0.17
(1,1715)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	3	0.17
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	2	0.17
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	9	0.17
(1,1549)	1:318:A:LEU:HA	1:382:A:LEU:HA	5	0.17
(1,1492)	1:314:A:MET:HB2	1:316:A:ASN:HA	8	0.17
(1,1492)	1:314:A:MET:HB3	1:316:A:ASN:HA	8	0.17
(1,1489)	1:314:A:MET:HB2	1:318:A:LEU:H	18	0.17
(1,1489)	1:314:A:MET:HB3	1:318:A:LEU:H	18	0.17
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD11	14	0.17
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD12	14	0.17
(1,1441)	1:313:A:PHE:HA	1:352:A:LEU:HD13	14	0.17
(1,1429)	1:312:A:GLN:HE21	1:336:A:ARG:HA	15	0.17
(1,1429)	1:312:A:GLN:HE22	1:336:A:ARG:HA	15	0.17
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	9	0.17
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	9	0.17
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	9	0.17
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	12	0.17
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	18	0.17
(1,1320)	1:302:A:GLN:HA	1:328:A:SER:HA	12	0.17
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD11	8	0.17
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD12	8	0.17
(1,1314)	1:302:A:GLN:HE21	1:332:A:LEU:HD13	8	0.17
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD11	8	0.17
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD12	8	0.17
(1,1314)	1:302:A:GLN:HE22	1:332:A:LEU:HD13	8	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	4	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	4	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	4	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	8	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	8	0.17
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	8	0.17
(1,1171)	1:298:A:LYS:HA	1:307:A:MET:H	7	0.17
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD2	13	0.17
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD3	13	0.17
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	2	0.17
(1,936)	1:284:A:ALA:HA	1:378:A:PHE:HZ	11	0.17
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	3	0.17
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	9	0.17
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	9	0.17
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	14	0.17
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	14	0.17
(1,751)	1:275:A:THR:HG21	1:325:A:ILE:HA	9	0.17
(1,751)	1:275:A:THR:HG22	1:325:A:ILE:HA	9	0.17
(1,751)	1:275:A:THR:HG23	1:325:A:ILE:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:275:A:THR:HB	1:325:A:ILE:HA	9	0.17
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	18	0.17
(1,666)	1:269:A:GLU:H	1:273:A:GLU:HA	6	0.17
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	7	0.17
(1,634)	1:267:A:ARG:HG2	1:274:A:TYR:H	1	0.17
(1,634)	1:267:A:ARG:HG3	1:274:A:TYR:H	1	0.17
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	18	0.17
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	19	0.17
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	3	0.17
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	16	0.17
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	16	0.17
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	20	0.17
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	13	0.17
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	13	0.17
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	13	0.17
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	13	0.17
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	13	0.17
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	13	0.17
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	6	0.17
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	6	0.17
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	6	0.17
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	6	0.17
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	6	0.17
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	6	0.17
(1,393)	1:252:A:HIS:HA	1:255:A:HIS:H	9	0.17
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	18	0.17
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	18	0.17
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	18	0.17
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	11	0.17
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	6	0.17
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	6	0.17
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG21	13	0.17
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG22	13	0.17
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG23	13	0.17
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	1	0.17
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	14	0.17
(3,2)	1:392:A:ASN:ND2	2:631:B:VAL:O	12	0.16
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD11	19	0.16
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD12	19	0.16
(1,3691)	1:385:A:GLY:H	2:629:B:LEU:HD13	19	0.16
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	10	0.16
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	10	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	10	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	10	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	10	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	10	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	10	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	10	0.16
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD21	20	0.16
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD22	20	0.16
(1,3690)	1:318:A:LEU:HD11	2:629:B:LEU:HD23	20	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD21	20	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD22	20	0.16
(1,3690)	1:318:A:LEU:HD12	2:629:B:LEU:HD23	20	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD21	20	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD22	20	0.16
(1,3690)	1:318:A:LEU:HD13	2:629:B:LEU:HD23	20	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	3	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	3	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	3	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	3	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	3	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	3	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	3	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	3	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	3	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD21	17	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD22	17	0.16
(1,3685)	1:457:A:VAL:HG21	2:606:B:LEU:HD23	17	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD21	17	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD22	17	0.16
(1,3685)	1:457:A:VAL:HG22	2:606:B:LEU:HD23	17	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD21	17	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD22	17	0.16
(1,3685)	1:457:A:VAL:HG23	2:606:B:LEU:HD23	17	0.16
(1,3615)	1:475:A:PHE:HD1	1:476:A:ASP:HB2	15	0.16
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	9	0.16
(1,3583)	1:474:A:GLU:HA	1:480:A:PHE:H	7	0.16
(1,3575)	1:473:A:THR:HB	1:480:A:PHE:H	10	0.16
(1,3525)	1:468:A:MET:HA	1:472:A:LEU:H	10	0.16
(1,3521)	1:467:A:TRP:HA	1:469:A:MET:H	17	0.16
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	3	0.16
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	3	0.16
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	9	0.16
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	9	0.16
(1,3220)	1:436:A:ASP:HA	1:463:A:ARG:HA	12	0.16
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	4	0.16
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	4	0.16
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	4	0.16
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	8	0.16
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	8	0.16
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	8	0.16
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	8	0.16
(1,3082)	1:428:A:GLU:HA	1:478:A:LYS:HA	11	0.16
(1,3062)	1:426:A:GLY:HA2	1:428:A:GLU:HA	7	0.16
(1,3062)	1:426:A:GLY:HA3	1:428:A:GLU:HA	7	0.16
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	18	0.16
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	18	0.16
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	18	0.16
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	18	0.16
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	18	0.16
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	18	0.16
(1,2969)	1:419:A:TYR:HE1	1:431:A:TYR:H	5	0.16
(1,2969)	1:419:A:TYR:HE2	1:431:A:TYR:H	5	0.16
(1,2939)	1:417:A:GLU:HA	1:420:A:VAL:HB	1	0.16
(1,2889)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	20	0.16
(1,2889)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	20	0.16
(1,2889)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	20	0.16
(1,2889)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	20	0.16
(1,2889)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	20	0.16
(1,2889)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	20	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	1	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	1	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	1	0.16
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	1	0.16
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	1	0.16
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	1	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	1	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	1	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	1	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	9	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	9	0.16
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	9	0.16
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	9	0.16
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	9	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	9	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	9	0.16
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	9	0.16
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD1	11	0.16
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	13	0.16
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	13	0.16
(1,2834)	1:407:A:THR:HG21	1:408:A:ASP:H	13	0.16
(1,2834)	1:407:A:THR:HG22	1:408:A:ASP:H	13	0.16
(1,2834)	1:407:A:THR:HG23	1:408:A:ASP:H	13	0.16
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG2	6	0.16
(1,2818)	1:406:A:HIS:HA	1:456:A:GLU:HG3	6	0.16
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	16	0.16
(1,2683)	1:401:A:ARG:HD2	1:413:A:THR:HA	19	0.16
(1,2683)	1:401:A:ARG:HD3	1:413:A:THR:HA	19	0.16
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD11	5	0.16
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD12	5	0.16
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD13	5	0.16
(1,2638)	1:398:A:LYS:HA	1:475:A:PHE:HZ	19	0.16
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	10	0.16
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	19	0.16
(1,2575)	1:393:A:GLN:HA	1:396:A:ILE:H	4	0.16
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD11	17	0.16
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD12	17	0.16
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD13	17	0.16
(1,2429)	1:383:A:LYS:HD2	1:462:A:ASP:HB2	9	0.16
(1,2429)	1:383:A:LYS:HD2	1:462:A:ASP:HB3	9	0.16
(1,2429)	1:383:A:LYS:HD3	1:462:A:ASP:HB2	9	0.16
(1,2429)	1:383:A:LYS:HD3	1:462:A:ASP:HB3	9	0.16
(1,2390)	1:381:A:VAL:HA	1:384:A:GLU:H	6	0.16
(1,2357)	1:379:A:GLY:H	1:382:A:LEU:H	8	0.16
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG21	9	0.16
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG22	9	0.16
(1,2320)	1:376:A:GLN:HE21	1:413:A:THR:HG23	9	0.16
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG21	9	0.16
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG22	9	0.16
(1,2320)	1:376:A:GLN:HE22	1:413:A:THR:HG23	9	0.16
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	13	0.16
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	3	0.16
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	15	0.16
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	17	0.16
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	8	0.16
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	8	0.16
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	8	0.16
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	13	0.16
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	13	0.16
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	13	0.16
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	15	0.16
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB2	4	0.16
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB3	4	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	18	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	18	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	18	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	20	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	20	0.16
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	20	0.16
(1,1984)	1:356:A:VAL:H	1:358:A:GLN:H	3	0.16
(1,1965)	1:355:A:ARG:H	1:358:A:GLN:H	3	0.16
(1,1951)	1:354:A:LYS:HA	1:358:A:GLN:H	20	0.16
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	4	0.16
(1,1824)	1:343:A:THR:HA	1:345:A:THR:HB	7	0.16
(1,1794)	1:340:A:GLN:HA	1:345:A:THR:HB	18	0.16
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	8	0.16
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	8	0.16
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	20	0.16
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	20	0.16
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	13	0.16
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD21	13	0.16
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD22	13	0.16
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD23	13	0.16
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD21	13	0.16
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD22	13	0.16
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD23	13	0.16
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD21	13	0.16
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD22	13	0.16
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD23	13	0.16
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	1	0.16
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	1	0.16
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	19	0.16
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	19	0.16
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	5	0.16
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	10	0.16
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	10	0.16
(1,1419)	1:312:A:GLN:HE21	1:340:A:GLN:H	18	0.16
(1,1419)	1:312:A:GLN:HE22	1:340:A:GLN:H	18	0.16
(1,1366)	1:307:A:MET:HE1	1:339:A:LEU:H	14	0.16
(1,1366)	1:307:A:MET:HE2	1:339:A:LEU:H	14	0.16
(1,1366)	1:307:A:MET:HE3	1:339:A:LEU:H	14	0.16
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	4	0.16
(1,1214)	1:299:A:LEU:H	1:307:A:MET:H	18	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	6	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	6	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	6	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	14	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	14	0.16
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	14	0.16
(1,1166)	1:298:A:LYS:HA	1:309:A:ASP:HA	15	0.16
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD2	2	0.16
(1,1158)	1:298:A:LYS:H	1:322:A:ARG:HD3	2	0.16
(1,1121)	1:297:A:LEU:HD11	1:314:A:MET:HA	20	0.16
(1,1121)	1:297:A:LEU:HD12	1:314:A:MET:HA	20	0.16
(1,1121)	1:297:A:LEU:HD13	1:314:A:MET:HA	20	0.16
(1,1089)	1:296:A:GLY:H	1:311:A:GLU:HA	15	0.16
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	11	0.16
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	8	0.16
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	8	0.16
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	8	0.16
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	8	0.16
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	13	0.16
(1,1050)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	13	0.16
(1,1035)	1:290:A:ASN:HA	1:292:A:ASP:H	5	0.16
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	10	0.16
(1,1028)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	10	0.16
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	8	0.16
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	8	0.16
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	8	0.16
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	8	0.16
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	8	0.16
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	8	0.16
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	6	0.16
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	7	0.16
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	7	0.16
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	3	0.16
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	4	0.16
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG2	2	0.16
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG3	2	0.16
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	3	0.16
(1,459)	1:258:A:ASN:HD21	1:282:A:SER:H	12	0.16
(1,459)	1:258:A:ASN:HD22	1:282:A:SER:H	12	0.16
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	9	0.16
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	9	0.16
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	9	0.16
(1,335)	1:250:A:TYR:HE1	1:281:A:PRO:HA	12	0.16
(1,335)	1:250:A:TYR:HE2	1:281:A:PRO:HA	12	0.16
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	4	0.16
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA2	14	0.16
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA3	14	0.16
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA2	14	0.16
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA3	14	0.16
(1,269)	1:247:A:LYS:HG2	1:263:A:TRP:HZ3	7	0.16
(1,269)	1:247:A:LYS:HG3	1:263:A:TRP:HZ3	7	0.16
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	5	0.16
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	16	0.16
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	16	0.16
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	19	0.16
(1,158)	1:238:A:LYS:HA	1:241:A:ILE:HB	4	0.16
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	2	0.16
(1,57)	1:234:A:TRP:HE1	1:326:A:ASP:H	1	0.16
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	14	0.15
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG11	7	0.15
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG12	7	0.15
(1,3669)	1:357:A:LEU:HD11	2:631:B:VAL:HG13	7	0.15
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG11	7	0.15
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG12	7	0.15
(1,3669)	1:357:A:LEU:HD12	2:631:B:VAL:HG13	7	0.15
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG11	7	0.15
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG12	7	0.15
(1,3669)	1:357:A:LEU:HD13	2:631:B:VAL:HG13	7	0.15
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB1	15	0.15
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB2	15	0.15
(1,3656)	1:450:A:LEU:HD11	2:609:B:ALA:HB3	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB1	15	0.15
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB2	15	0.15
(1,3656)	1:450:A:LEU:HD12	2:609:B:ALA:HB3	15	0.15
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB1	15	0.15
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB2	15	0.15
(1,3656)	1:450:A:LEU:HD13	2:609:B:ALA:HB3	15	0.15
(1,3592)	1:474:A:GLU:HG2	1:478:A:LYS:HA	4	0.15
(1,3592)	1:474:A:GLU:HG3	1:478:A:LYS:HA	4	0.15
(1,3578)	1:473:A:THR:HB	1:479:A:PRO:HA	10	0.15
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	10	0.15
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	18	0.15
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	9	0.15
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	4	0.15
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	4	0.15
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	4	0.15
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	4	0.15
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	15	0.15
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	15	0.15
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	19	0.15
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	19	0.15
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	19	0.15
(1,3333)	1:445:A:PRO:HG2	1:446:A:HIS:H	6	0.15
(1,3333)	1:445:A:PRO:HG3	1:446:A:HIS:H	6	0.15
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB2	20	0.15
(1,3280)	1:441:A:ALA:H	1:461:A:SER:HB3	20	0.15
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	5	0.15
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	10	0.15
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	3	0.15
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	3	0.15
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	3	0.15
(1,3142)	1:431:A:TYR:HA	1:480:A:PHE:HA	10	0.15
(1,3136)	1:431:A:TYR:HA	1:482:A:SER:HA	1	0.15
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	1	0.15
(1,3050)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	1	0.15
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	1	0.15
(1,3050)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	1	0.15
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE21	3	0.15
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE22	3	0.15
(1,3012)	1:422:A:ARG:HB2	1:456:A:GLU:HB2	15	0.15
(1,3012)	1:422:A:ARG:HB2	1:456:A:GLU:HB3	15	0.15
(1,3012)	1:422:A:ARG:HB3	1:456:A:GLU:HB2	15	0.15
(1,3012)	1:422:A:ARG:HB3	1:456:A:GLU:HB3	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2938)	1:417:A:GLU:HA	1:420:A:VAL:H	10	0.15
(1,2859)	1:410:A:SER:HB2	1:438:A:TYR:HD1	2	0.15
(1,2859)	1:410:A:SER:HB2	1:438:A:TYR:HD2	2	0.15
(1,2859)	1:410:A:SER:HB3	1:438:A:TYR:HD1	2	0.15
(1,2859)	1:410:A:SER:HB3	1:438:A:TYR:HD2	2	0.15
(1,2845)	1:409:A:SER:H	1:442:A:LYS:HE2	17	0.15
(1,2845)	1:409:A:SER:H	1:442:A:LYS:HE3	17	0.15
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	17	0.15
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	17	0.15
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	17	0.15
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	17	0.15
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	17	0.15
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	17	0.15
(1,2777)	1:404:A:SER:H	1:406:A:HIS:H	5	0.15
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	5	0.15
(1,2733)	1:403:A:ALA:H	1:414:A:VAL:H	13	0.15
(1,2639)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	16	0.15
(1,2639)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	16	0.15
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	2	0.15
(1,2498)	1:386:A:PRO:HA	1:393:A:GLN:HA	20	0.15
(1,2453)	1:384:A:GLU:HA	1:467:A:TRP:HZ3	10	0.15
(1,2452)	1:384:A:GLU:HA	1:467:A:TRP:HH2	5	0.15
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	5	0.15
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	5	0.15
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	13	0.15
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	13	0.15
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	19	0.15
(1,2259)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	19	0.15
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	1	0.15
(1,2144)	1:365:A:LYS:HA	1:367:A:ASP:H	12	0.15
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	17	0.15
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	17	0.15
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	18	0.15
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	18	0.15
(1,2074)	1:361:A:GLU:HA	1:365:A:LYS:H	9	0.15
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	2	0.15
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	2	0.15
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	2	0.15
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	9	0.15
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	9	0.15
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	9	0.15
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	14	0.15
(1,1993)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	14	0.15
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	14	0.15
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	14	0.15
(1,1993)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	14	0.15
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD21	10	0.15
(1,1855)	1:346:A:ARG:HA	1:350:A:ASN:HD22	10	0.15
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	14	0.15
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	14	0.15
(1,1794)	1:340:A:GLN:HA	1:345:A:THR:HB	2	0.15
(1,1780)	1:339:A:LEU:HA	1:345:A:THR:H	2	0.15
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD11	18	0.15
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD12	18	0.15
(1,1738)	1:335:A:SER:H	1:338:A:ILE:HD13	18	0.15
(1,1737)	1:335:A:SER:H	1:338:A:ILE:HB	16	0.15
(1,1644)	1:325:A:ILE:HD11	1:327:A:SER:H	10	0.15
(1,1644)	1:325:A:ILE:HD12	1:327:A:SER:H	10	0.15
(1,1644)	1:325:A:ILE:HD13	1:327:A:SER:H	10	0.15
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	14	0.15
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	14	0.15
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	5	0.15
(1,1554)	1:318:A:LEU:HD21	1:374:A:PHE:HZ	19	0.15
(1,1554)	1:318:A:LEU:HD22	1:374:A:PHE:HZ	19	0.15
(1,1554)	1:318:A:LEU:HD23	1:374:A:PHE:HZ	19	0.15
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	5	0.15
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	5	0.15
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	1	0.15
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	1	0.15
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	3	0.15
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	3	0.15
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	10	0.15
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	10	0.15
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	10	0.15
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD11	13	0.15
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD12	13	0.15
(1,1243)	1:300:A:TYR:H	1:325:A:ILE:HD13	13	0.15
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	6	0.15
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	10	0.15
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	10	0.15
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	9	0.15
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	19	0.15
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	3	0.15
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	8	0.15
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	8	0.15
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	12	0.15
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	12	0.15
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	17	0.15
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	17	0.15
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	3	0.15
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	6	0.15
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	6	0.15
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	6	0.15
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	12	0.15
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	12	0.15
(1,575)	1:264:A:SER:HB2	1:356:A:VAL:HA	1	0.15
(1,575)	1:264:A:SER:HB3	1:356:A:VAL:HA	1	0.15
(1,566)	1:263:A:TRP:HE1	1:265:A:HIS:HB2	1	0.15
(1,566)	1:263:A:TRP:HE1	1:265:A:HIS:HB3	1	0.15
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	15	0.15
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	14	0.15
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	10	0.15
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	10	0.15
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	2	0.15
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	2	0.15
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	18	0.15
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	6	0.15
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	4	0.15
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	4	0.15
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	6	0.15
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	1	0.15
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	1	0.15
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	1	0.15
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	1	0.15
(1,266)	1:247:A:LYS:HE2	1:263:A:TRP:HH2	1	0.15
(1,266)	1:247:A:LYS:HE3	1:263:A:TRP:HH2	1	0.15
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD21	1	0.15
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD22	1	0.15
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD21	1	0.15
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD22	1	0.15
(1,147)	1:238:A:LYS:HD2	1:266:A:ASN:HD21	1	0.15
(1,147)	1:238:A:LYS:HD2	1:266:A:ASN:HD22	1	0.15
(1,147)	1:238:A:LYS:HD3	1:266:A:ASN:HD21	1	0.15
(1,147)	1:238:A:LYS:HD3	1:266:A:ASN:HD22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	2	0.15
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	2	0.15
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	9	0.15
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	4	0.15
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	4	0.15
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	3	0.15
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	3	0.15
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	3	0.15
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	3	0.15
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	3	0.15
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	3	0.15
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	11	0.14
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	11	0.14
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	13	0.14
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	13	0.14
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	1	0.14
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	1	0.14
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	1	0.14
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	1	0.14
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	1	0.14
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	1	0.14
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	1	0.14
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	1	0.14
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	1	0.14
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE1	5	0.14
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE2	5	0.14
(1,3682)	1:467:A:TRP:HE3	2:624:B:MET:HE3	5	0.14
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB1	14	0.14
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB2	14	0.14
(1,3676)	1:457:A:VAL:HG21	2:609:B:ALA:HB3	14	0.14
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB1	14	0.14
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB2	14	0.14
(1,3676)	1:457:A:VAL:HG22	2:609:B:ALA:HB3	14	0.14
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB1	14	0.14
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB2	14	0.14
(1,3676)	1:457:A:VAL:HG23	2:609:B:ALA:HB3	14	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD21	13	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD22	13	0.14
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD23	13	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD21	13	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD22	13	0.14
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD23	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD21	13	0.14
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD22	13	0.14
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD23	13	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD11	13	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD12	13	0.14
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD13	13	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD11	13	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD12	13	0.14
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD13	13	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD11	13	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD12	13	0.14
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD13	13	0.14
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	3	0.14
(1,3605)	1:475:A:PHE:H	1:479:A:PRO:HA	4	0.14
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	16	0.14
(1,3557)	1:471:A:TYR:H	1:473:A:THR:H	15	0.14
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	12	0.14
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	12	0.14
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	12	0.14
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	12	0.14
(1,3521)	1:467:A:TRP:HA	1:469:A:MET:H	5	0.14
(1,3521)	1:467:A:TRP:HA	1:469:A:MET:H	14	0.14
(1,3464)	1:462:A:ASP:H	1:465:A:ASP:H	2	0.14
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG21	16	0.14
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG22	16	0.14
(1,3422)	1:455:A:ILE:HB	1:457:A:VAL:HG23	16	0.14
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	3	0.14
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	3	0.14
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	3	0.14
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	9	0.14
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	9	0.14
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB2	15	0.14
(1,3288)	1:441:A:ALA:HA	1:444:A:SER:HB3	15	0.14
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	2	0.14
(1,3271)	1:440:A:ALA:HA	1:444:A:SER:H	5	0.14
(1,3197)	1:434:A:THR:HB	1:466:A:GLU:H	14	0.14
(1,3181)	1:433:A:ILE:H	1:460:A:LEU:H	3	0.14
(1,3181)	1:433:A:ILE:H	1:460:A:LEU:H	13	0.14
(1,3142)	1:431:A:TYR:HA	1:480:A:PHE:HA	16	0.14
(1,3116)	1:430:A:ILE:HB	1:480:A:PHE:HA	3	0.14
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	6	0.14
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	6	0.14
(1,3101)	1:429:A:LYS:HA	1:478:A:LYS:HA	16	0.14
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	1	0.14
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	1	0.14
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	9	0.14
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	9	0.14
(1,3028)	1:423:A:MET:HE1	1:429:A:LYS:H	6	0.14
(1,3028)	1:423:A:MET:HE2	1:429:A:LYS:H	6	0.14
(1,3028)	1:423:A:MET:HE3	1:429:A:LYS:H	6	0.14
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD1	12	0.14
(1,3024)	1:423:A:MET:HE1	1:431:A:TYR:HD2	12	0.14
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD1	12	0.14
(1,3024)	1:423:A:MET:HE2	1:431:A:TYR:HD2	12	0.14
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD1	12	0.14
(1,3024)	1:423:A:MET:HE3	1:431:A:TYR:HD2	12	0.14
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD2	4	0.14
(1,2980)	1:419:A:TYR:HA	1:422:A:ARG:HD3	4	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	3	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	3	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	4	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	4	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	18	0.14
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	18	0.14
(1,2828)	1:407:A:THR:HB	1:409:A:SER:H	5	0.14
(1,2714)	1:402:A:PHE:HA	1:412:A:GLN:HA	13	0.14
(1,2711)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	17	0.14
(1,2711)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	17	0.14
(1,2711)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	17	0.14
(1,2711)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	17	0.14
(1,2711)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	17	0.14
(1,2711)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	17	0.14
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	1	0.14
(1,2708)	1:402:A:PHE:H	1:414:A:VAL:H	5	0.14
(1,2680)	1:401:A:ARG:HD2	1:414:A:VAL:H	19	0.14
(1,2680)	1:401:A:ARG:HD3	1:414:A:VAL:H	19	0.14
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD11	13	0.14
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD12	13	0.14
(1,2655)	1:399:A:LEU:H	1:416:A:LEU:HD13	13	0.14
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD11	20	0.14
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD12	20	0.14
(1,2534)	1:389:A:ASP:HA	1:396:A:ILE:HD13	20	0.14
(1,2343)	1:378:A:PHE:HA	1:381:A:VAL:HB	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	12	0.14
(1,2278)	1:375:A:TRP:HD1	1:413:A:THR:HA	9	0.14
(1,2170)	1:368:A:ALA:HA	1:371:A:TYR:HB2	9	0.14
(1,2170)	1:368:A:ALA:HA	1:371:A:TYR:HB3	9	0.14
(1,2141)	1:365:A:LYS:HA	1:368:A:ALA:HA	20	0.14
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	7	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	8	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	8	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	8	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	13	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	13	0.14
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	13	0.14
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	19	0.14
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	19	0.14
(1,1955)	1:354:A:LYS:HA	1:357:A:LEU:HB2	8	0.14
(1,1955)	1:354:A:LYS:HA	1:357:A:LEU:HB3	8	0.14
(1,1952)	1:354:A:LYS:HB2	1:358:A:GLN:H	11	0.14
(1,1952)	1:354:A:LYS:HB3	1:358:A:GLN:H	11	0.14
(1,1952)	1:354:A:LYS:HB2	1:358:A:GLN:H	15	0.14
(1,1952)	1:354:A:LYS:HB3	1:358:A:GLN:H	15	0.14
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	5	0.14
(1,1903)	1:350:A:ASN:HA	1:354:A:LYS:H	12	0.14
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	13	0.14
(1,1856)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	13	0.14
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	13	0.14
(1,1856)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	13	0.14
(1,1852)	1:345:A:THR:HB	1:346:A:ARG:H	16	0.14
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	15	0.14
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	15	0.14
(1,1758)	1:337:A:GLU:HA	1:341:A:ASP:H	16	0.14
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	10	0.14
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	10	0.14
(1,1644)	1:325:A:ILE:HD11	1:327:A:SER:H	17	0.14
(1,1644)	1:325:A:ILE:HD12	1:327:A:SER:H	17	0.14
(1,1644)	1:325:A:ILE:HD13	1:327:A:SER:H	17	0.14
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	4	0.14
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	4	0.14
(1,1617)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	4	0.14
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	4	0.14
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	4	0.14
(1,1617)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	4	0.14
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	4	0.14
(1,1617)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	4	0.14
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	19	0.14
(1,1541)	1:317:A:TYR:HA	1:320:A:PHE:HD1	8	0.14
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG2	4	0.14
(1,1520)	1:316:A:ASN:HB2	1:388:A:GLU:HG3	4	0.14
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG2	4	0.14
(1,1520)	1:316:A:ASN:HB3	1:388:A:GLU:HG3	4	0.14
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HG2	13	0.14
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HG3	13	0.14
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	8	0.14
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	8	0.14
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	8	0.14
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	18	0.14
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	18	0.14
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	18	0.14
(1,1372)	1:307:A:MET:HE1	1:335:A:SER:H	18	0.14
(1,1372)	1:307:A:MET:HE2	1:335:A:SER:H	18	0.14
(1,1372)	1:307:A:MET:HE3	1:335:A:SER:H	18	0.14
(1,1319)	1:302:A:GLN:H	1:328:A:SER:HA	1	0.14
(1,1196)	1:299:A:LEU:HA	1:325:A:ILE:H	4	0.14
(1,1196)	1:299:A:LEU:HA	1:325:A:ILE:H	7	0.14
(1,1196)	1:299:A:LEU:HA	1:325:A:ILE:H	11	0.14
(1,1159)	1:298:A:LYS:HG2	1:322:A:ARG:HD2	15	0.14
(1,1159)	1:298:A:LYS:HG2	1:322:A:ARG:HD3	15	0.14
(1,1159)	1:298:A:LYS:HG3	1:322:A:ARG:HD2	15	0.14
(1,1159)	1:298:A:LYS:HG3	1:322:A:ARG:HD3	15	0.14
(1,1139)	1:297:A:LEU:HA	1:309:A:ASP:HA	3	0.14
(1,1090)	1:296:A:GLY:HA2	1:311:A:GLU:HA	15	0.14
(1,1090)	1:296:A:GLY:HA3	1:311:A:GLU:HA	15	0.14
(1,1080)	1:296:A:GLY:H	1:319:A:ARG:HA	17	0.14
(1,1023)	1:289:A:TRP:HH2	1:381:A:VAL:HA	16	0.14
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	3	0.14
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	3	0.14
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	8	0.14
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	8	0.14
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	14	0.14
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	16	0.14
(1,647)	1:268:A:VAL:H	1:274:A:TYR:H	1	0.14
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	5	0.14
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	5	0.14
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	14	0.14
(1,576)	1:264:A:SER:HB2	1:356:A:VAL:HG21	11	0.14
(1,576)	1:264:A:SER:HB2	1:356:A:VAL:HG22	11	0.14
(1,576)	1:264:A:SER:HB2	1:356:A:VAL:HG23	11	0.14
(1,576)	1:264:A:SER:HB3	1:356:A:VAL:HG21	11	0.14
(1,576)	1:264:A:SER:HB3	1:356:A:VAL:HG22	11	0.14
(1,576)	1:264:A:SER:HB3	1:356:A:VAL:HG23	11	0.14
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	3	0.14
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	9	0.14
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	9	0.14
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	18	0.14
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	18	0.14
(1,539)	1:262:A:THR:HG21	1:280:A:ILE:HB	5	0.14
(1,539)	1:262:A:THR:HG22	1:280:A:ILE:HB	5	0.14
(1,539)	1:262:A:THR:HG23	1:280:A:ILE:HB	5	0.14
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	3	0.14
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	3	0.14
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	19	0.14
(1,467)	1:259:A:ASP:HB2	1:261:A:LEU:HA	10	0.14
(1,467)	1:259:A:ASP:HB3	1:261:A:LEU:HA	10	0.14
(1,467)	1:259:A:ASP:HB2	1:261:A:LEU:HA	11	0.14
(1,467)	1:259:A:ASP:HB3	1:261:A:LEU:HA	11	0.14
(1,418)	1:253:A:ILE:HD11	1:255:A:HIS:H	8	0.14
(1,418)	1:253:A:ILE:HD12	1:255:A:HIS:H	8	0.14
(1,418)	1:253:A:ILE:HD13	1:255:A:HIS:H	8	0.14
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	16	0.14
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE2	19	0.14
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE3	19	0.14
(1,269)	1:247:A:LYS:HG2	1:263:A:TRP:HZ3	6	0.14
(1,269)	1:247:A:LYS:HG3	1:263:A:TRP:HZ3	6	0.14
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	16	0.14
(1,149)	1:238:A:LYS:HA	1:265:A:HIS:HE1	7	0.14
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	1	0.14
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	10	0.14
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	1	0.14
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	1	0.14
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	1	0.14
(1,44)	1:233:A:LEU:HD11	1:242:A:THR:H	3	0.14
(1,44)	1:233:A:LEU:HD12	1:242:A:THR:H	3	0.14
(1,44)	1:233:A:LEU:HD13	1:242:A:THR:H	3	0.14
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	10	0.14
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	10	0.14
(3,1)	1:392:A:ASN:ND2	2:630:B:LEU:O	8	0.13
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD21	3	0.13
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD22	3	0.13
(1,3671)	1:318:A:LEU:HD21	2:628:B:LEU:HD23	3	0.13
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD21	3	0.13
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD22	3	0.13
(1,3671)	1:318:A:LEU:HD22	2:628:B:LEU:HD23	3	0.13
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD21	3	0.13
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD22	3	0.13
(1,3671)	1:318:A:LEU:HD23	2:628:B:LEU:HD23	3	0.13
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD11	3	0.13
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD12	3	0.13
(1,3671)	1:318:A:LEU:HD11	2:628:B:LEU:HD13	3	0.13
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD11	3	0.13
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD12	3	0.13
(1,3671)	1:318:A:LEU:HD12	2:628:B:LEU:HD13	3	0.13
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD11	3	0.13
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD12	3	0.13
(1,3671)	1:318:A:LEU:HD13	2:628:B:LEU:HD13	3	0.13
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	10	0.13
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	15	0.13
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB2	1	0.13
(1,3526)	1:468:A:MET:HG2	1:472:A:LEU:HB3	1	0.13
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB2	1	0.13
(1,3526)	1:468:A:MET:HG3	1:472:A:LEU:HB3	1	0.13
(1,3481)	1:464:A:ILE:HA	1:468:A:MET:H	19	0.13
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG21	1	0.13
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG22	1	0.13
(1,3396)	1:451:A:ARG:HA	1:457:A:VAL:HG23	1	0.13
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG21	1	0.13
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG22	1	0.13
(1,3395)	1:451:A:ARG:H	1:457:A:VAL:HG23	1	0.13
(1,3386)	1:450:A:LEU:HA	1:454:A:GLY:H	11	0.13
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	19	0.13
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	19	0.13
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	19	0.13
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	19	0.13
(1,3265)	1:439:A:ALA:HA	1:442:A:LYS:HD2	12	0.13
(1,3265)	1:439:A:ALA:HA	1:442:A:LYS:HD3	12	0.13
(1,3220)	1:436:A:ASP:HA	1:463:A:ARG:HA	6	0.13
(1,3195)	1:434:A:THR:H	1:482:A:SER:HA	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	1	0.13
(1,3179)	1:433:A:ILE:HA	1:482:A:SER:HA	13	0.13
(1,3152)	1:431:A:TYR:HB2	1:456:A:GLU:H	6	0.13
(1,3152)	1:431:A:TYR:HB3	1:456:A:GLU:H	6	0.13
(1,3143)	1:431:A:TYR:H	1:458:A:LEU:H	5	0.13
(1,3143)	1:431:A:TYR:H	1:458:A:LEU:H	8	0.13
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD11	19	0.13
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD12	19	0.13
(1,3110)	1:429:A:LYS:HA	1:430:A:ILE:HD13	19	0.13
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	7	0.13
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	7	0.13
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	7	0.13
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	7	0.13
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG2	12	0.13
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG3	12	0.13
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG2	12	0.13
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG3	12	0.13
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	12	0.13
(1,3068)	1:427:A:GLN:HE21	1:456:A:GLU:H	14	0.13
(1,3068)	1:427:A:GLN:HE22	1:456:A:GLU:H	14	0.13
(1,3047)	1:424:A:LYS:H	1:427:A:GLN:HB2	5	0.13
(1,3047)	1:424:A:LYS:H	1:427:A:GLN:HB3	5	0.13
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE21	17	0.13
(1,3034)	1:423:A:MET:HA	1:427:A:GLN:HE22	17	0.13
(1,3023)	1:423:A:MET:HE1	1:431:A:TYR:H	7	0.13
(1,3023)	1:423:A:MET:HE2	1:431:A:TYR:H	7	0.13
(1,3023)	1:423:A:MET:HE3	1:431:A:TYR:H	7	0.13
(1,2935)	1:417:A:GLU:HB2	1:421:A:SER:H	4	0.13
(1,2935)	1:417:A:GLU:HB3	1:421:A:SER:H	4	0.13
(1,2934)	1:417:A:GLU:HA	1:421:A:SER:H	6	0.13
(1,2896)	1:415:A:SER:H	1:418:A:ASP:H	15	0.13
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG21	5	0.13
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG22	5	0.13
(1,2868)	1:411:A:ALA:HB1	1:413:A:THR:HG23	5	0.13
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG21	5	0.13
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG22	5	0.13
(1,2868)	1:411:A:ALA:HB2	1:413:A:THR:HG23	5	0.13
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG21	5	0.13
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG22	5	0.13
(1,2868)	1:411:A:ALA:HB3	1:413:A:THR:HG23	5	0.13
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	1	0.13
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	14	0.13
(1,2680)	1:401:A:ARG:HD2	1:414:A:VAL:H	7	0.13
(1,2680)	1:401:A:ARG:HD3	1:414:A:VAL:H	7	0.13
(1,2680)	1:401:A:ARG:HD2	1:414:A:VAL:H	8	0.13
(1,2680)	1:401:A:ARG:HD3	1:414:A:VAL:H	8	0.13
(1,2645)	1:398:A:LYS:HA	1:416:A:LEU:H	2	0.13
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	17	0.13
(1,2643)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	17	0.13
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	17	0.13
(1,2643)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	17	0.13
(1,2601)	1:395:A:ALA:HA	1:398:A:LYS:H	1	0.13
(1,2563)	1:393:A:GLN:HE21	1:474:A:GLU:H	1	0.13
(1,2563)	1:393:A:GLN:HE22	1:474:A:GLU:H	1	0.13
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD11	8	0.13
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD12	8	0.13
(1,2557)	1:392:A:ASN:H	1:396:A:ILE:HD13	8	0.13
(1,2502)	1:386:A:PRO:HA	1:389:A:ASP:H	8	0.13
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB2	11	0.13
(1,2482)	1:386:A:PRO:HB2	1:471:A:TYR:HB3	11	0.13
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB2	11	0.13
(1,2482)	1:386:A:PRO:HB3	1:471:A:TYR:HB3	11	0.13
(1,2432)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	14	0.13
(1,2432)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	14	0.13
(1,2191)	1:370:A:LYS:HA	1:373:A:THR:HB	8	0.13
(1,2177)	1:369:A:GLU:HG2	1:373:A:THR:H	20	0.13
(1,2177)	1:369:A:GLU:HG3	1:373:A:THR:H	20	0.13
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	20	0.13
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	20	0.13
(1,2075)	1:361:A:GLU:HG2	1:365:A:LYS:HE2	10	0.13
(1,2075)	1:361:A:GLU:HG2	1:365:A:LYS:HE3	10	0.13
(1,2075)	1:361:A:GLU:HG3	1:365:A:LYS:HE2	10	0.13
(1,2075)	1:361:A:GLU:HG3	1:365:A:LYS:HE3	10	0.13
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	15	0.13
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	18	0.13
(1,2049)	1:360:A:LEU:HD21	1:364:A:ALA:H	11	0.13
(1,2049)	1:360:A:LEU:HD22	1:364:A:ALA:H	11	0.13
(1,2049)	1:360:A:LEU:HD23	1:364:A:ALA:H	11	0.13
(1,2009)	1:358:A:GLN:HA	1:361:A:GLU:H	1	0.13
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD11	14	0.13
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD12	14	0.13
(1,1991)	1:357:A:LEU:HA	1:399:A:LEU:HD13	14	0.13
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE21	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:355:A:ARG:HA	1:358:A:GLN:HE22	5	0.13
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB2	3	0.13
(1,1967)	1:355:A:ARG:HA	1:358:A:GLN:HB3	3	0.13
(1,1931)	1:352:A:LEU:HA	1:355:A:ARG:HD2	3	0.13
(1,1931)	1:352:A:LEU:HA	1:355:A:ARG:HD3	3	0.13
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	14	0.13
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	12	0.13
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	12	0.13
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	6	0.13
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	6	0.13
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	11	0.13
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	11	0.13
(1,1786)	1:339:A:LEU:HA	1:342:A:SER:H	13	0.13
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	7	0.13
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	7	0.13
(1,1554)	1:318:A:LEU:HD21	1:374:A:PHE:HZ	2	0.13
(1,1554)	1:318:A:LEU:HD22	1:374:A:PHE:HZ	2	0.13
(1,1554)	1:318:A:LEU:HD23	1:374:A:PHE:HZ	2	0.13
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	14	0.13
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	14	0.13
(1,1499)	1:315:A:PRO:HD2	1:353:A:THR:HA	10	0.13
(1,1499)	1:315:A:PRO:HD3	1:353:A:THR:HA	10	0.13
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG2	1	0.13
(1,1496)	1:315:A:PRO:HB2	1:388:A:GLU:HG3	1	0.13
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG2	1	0.13
(1,1496)	1:315:A:PRO:HB3	1:388:A:GLU:HG3	1	0.13
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	17	0.13
(1,1417)	1:312:A:GLN:HA	1:345:A:THR:HG21	1	0.13
(1,1417)	1:312:A:GLN:HA	1:345:A:THR:HG22	1	0.13
(1,1417)	1:312:A:GLN:HA	1:345:A:THR:HG23	1	0.13
(1,1381)	1:307:A:MET:HB2	1:308:A:ASP:H	16	0.13
(1,1381)	1:307:A:MET:HB3	1:308:A:ASP:H	16	0.13
(1,1351)	1:305:A:PHE:HZ	1:307:A:MET:HA	14	0.13
(1,1317)	1:302:A:GLN:H	1:329:A:ASP:H	10	0.13
(1,1254)	1:300:A:TYR:HA	1:306:A:ILE:HB	17	0.13
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	18	0.13
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	18	0.13
(1,1214)	1:299:A:LEU:H	1:307:A:MET:H	7	0.13
(1,1139)	1:297:A:LEU:HA	1:309:A:ASP:HA	15	0.13
(1,1090)	1:296:A:GLY:HA2	1:311:A:GLU:HA	3	0.13
(1,1090)	1:296:A:GLY:HA3	1:311:A:GLU:HA	3	0.13
(1,1007)	1:288:A:MET:HE1	1:320:A:PHE:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:288:A:MET:HE2	1:320:A:PHE:HA	15	0.13
(1,1007)	1:288:A:MET:HE3	1:320:A:PHE:HA	15	0.13
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	10	0.13
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	10	0.13
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	13	0.13
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	16	0.13
(1,878)	1:280:A:ILE:HA	1:322:A:ARG:HB2	2	0.13
(1,878)	1:280:A:ILE:HA	1:322:A:ARG:HB3	2	0.13
(1,781)	1:277:A:LEU:H	1:324:A:LEU:H	11	0.13
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	11	0.13
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	11	0.13
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	20	0.13
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	20	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	19	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	19	0.13
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	1	0.13
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	1	0.13
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	6	0.13
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	6	0.13
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	8	0.13
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	14	0.13
(1,541)	1:262:A:THR:H	1:279:A:TYR:HA	12	0.13
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB2	5	0.13
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB3	5	0.13
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB2	5	0.13
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB3	5	0.13
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB2	5	0.13
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB3	5	0.13
(1,403)	1:253:A:ILE:HB	1:323:A:GLY:HA2	18	0.13
(1,403)	1:253:A:ILE:HB	1:323:A:GLY:HA3	18	0.13
(1,370)	1:251:A:LYS:HE2	1:259:A:ASP:H	17	0.13
(1,370)	1:251:A:LYS:HE3	1:259:A:ASP:H	17	0.13
(1,339)	1:250:A:TYR:HE1	1:280:A:ILE:HA	13	0.13
(1,339)	1:250:A:TYR:HE2	1:280:A:ILE:HA	13	0.13
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	19	0.13
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	18	0.13
(1,211)	1:243:A:ASP:HA	1:246:A:TYR:H	3	0.13
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	7	0.13
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	13	0.13
(1,160)	1:238:A:LYS:HA	1:241:A:ILE:HD11	5	0.13
(1,160)	1:238:A:LYS:HA	1:241:A:ILE:HD12	5	0.13
(1,160)	1:238:A:LYS:HA	1:241:A:ILE:HD13	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:237:A:ASN:HD21	1:239:A:SER:HB2	5	0.13
(1,140)	1:237:A:ASN:HD21	1:239:A:SER:HB3	5	0.13
(1,140)	1:237:A:ASN:HD22	1:239:A:SER:HB2	5	0.13
(1,140)	1:237:A:ASN:HD22	1:239:A:SER:HB3	5	0.13
(1,92)	1:234:A:TRP:HZ3	1:249:A:PHE:HZ	17	0.13
(1,66)	1:234:A:TRP:HZ2	1:304:A:VAL:H	6	0.13
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	7	0.13
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	7	0.13
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	7	0.13
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	11	0.13
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB2	19	0.12
(2,13)	1:442:A:LYS:H	1:461:A:SER:HB3	19	0.12
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	6	0.12
(1,3615)	1:475:A:PHE:HD2	1:476:A:ASP:HB3	12	0.12
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	9	0.12
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	9	0.12
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	5	0.12
(1,3464)	1:462:A:ASP:H	1:465:A:ASP:H	4	0.12
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	2	0.12
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	2	0.12
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	2	0.12
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG11	20	0.12
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG12	20	0.12
(1,3344)	1:447:A:LEU:HA	1:457:A:VAL:HG13	20	0.12
(1,3276)	1:440:A:ALA:HA	1:442:A:LYS:H	9	0.12
(1,3230)	1:437:A:SER:HA	1:441:A:ALA:H	2	0.12
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	1	0.12
(1,3139)	1:431:A:TYR:HA	1:481:A:GLN:H	16	0.12
(1,3137)	1:431:A:TYR:HB2	1:482:A:SER:HA	12	0.12
(1,3137)	1:431:A:TYR:HB3	1:482:A:SER:HA	12	0.12
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG2	1	0.12
(1,3100)	1:429:A:LYS:HG2	1:479:A:PRO:HG3	1	0.12
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG2	1	0.12
(1,3100)	1:429:A:LYS:HG3	1:479:A:PRO:HG3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3069)	1:427:A:GLN:HE21	1:455:A:ILE:HA	8	0.12
(1,3069)	1:427:A:GLN:HE22	1:455:A:ILE:HA	8	0.12
(1,3062)	1:426:A:GLY:HA2	1:428:A:GLU:HA	13	0.12
(1,3062)	1:426:A:GLY:HA3	1:428:A:GLU:HA	13	0.12
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	15	0.12
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	15	0.12
(1,3022)	1:423:A:MET:HA	1:456:A:GLU:H	13	0.12
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD1	7	0.12
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	5	0.12
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	5	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	8	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	8	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	11	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	11	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE2	19	0.12
(1,2839)	1:408:A:ASP:HA	1:442:A:LYS:HE3	19	0.12
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD2	14	0.12
(1,2820)	1:406:A:HIS:HA	1:422:A:ARG:HD3	14	0.12
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG2	16	0.12
(1,2807)	1:405:A:THR:HG21	1:442:A:LYS:HG3	16	0.12
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG2	16	0.12
(1,2807)	1:405:A:THR:HG22	1:442:A:LYS:HG3	16	0.12
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG2	16	0.12
(1,2807)	1:405:A:THR:HG23	1:442:A:LYS:HG3	16	0.12
(1,2806)	1:405:A:THR:HG21	1:442:A:LYS:HA	17	0.12
(1,2806)	1:405:A:THR:HG22	1:442:A:LYS:HA	17	0.12
(1,2806)	1:405:A:THR:HG23	1:442:A:LYS:HA	17	0.12
(1,2795)	1:405:A:THR:H	1:457:A:VAL:HB	3	0.12
(1,2734)	1:403:A:ALA:HA	1:414:A:VAL:H	10	0.12
(1,2713)	1:402:A:PHE:H	1:412:A:GLN:HA	1	0.12
(1,2697)	1:402:A:PHE:HD1	1:461:A:SER:H	2	0.12
(1,2697)	1:402:A:PHE:HD2	1:461:A:SER:H	2	0.12
(1,2697)	1:402:A:PHE:HD1	1:461:A:SER:H	5	0.12
(1,2697)	1:402:A:PHE:HD2	1:461:A:SER:H	5	0.12
(1,2683)	1:401:A:ARG:HD2	1:413:A:THR:HA	8	0.12
(1,2683)	1:401:A:ARG:HD3	1:413:A:THR:HA	8	0.12
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD11	16	0.12
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD12	16	0.12
(1,2541)	1:390:A:PHE:HA	1:396:A:ILE:HD13	16	0.12
(1,2529)	1:388:A:GLU:H	1:390:A:PHE:H	4	0.12
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD2	2	0.12
(1,2378)	1:380:A:LEU:HA	1:383:A:LYS:HD3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2374)	1:380:A:LEU:HA	1:384:A:GLU:H	4	0.12
(1,2292)	1:375:A:TRP:HE3	1:400:A:LEU:HA	10	0.12
(1,2229)	1:372:A:GLN:HE21	1:376:A:GLN:H	8	0.12
(1,2229)	1:372:A:GLN:HE22	1:376:A:GLN:H	8	0.12
(1,2207)	1:371:A:TYR:HD2	1:375:A:TRP:H	14	0.12
(1,2168)	1:368:A:ALA:HA	1:371:A:TYR:H	9	0.12
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB2	9	0.12
(1,2107)	1:363:A:LEU:HA	1:367:A:ASP:HB3	9	0.12
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	5	0.12
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	5	0.12
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	6	0.12
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	6	0.12
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	13	0.12
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	13	0.12
(1,1596)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	17	0.12
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE1	11	0.12
(1,1542)	1:317:A:TYR:HA	1:320:A:PHE:HE2	11	0.12
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	2	0.12
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	2	0.12
(1,1530)	1:317:A:TYR:HB2	1:388:A:GLU:H	7	0.12
(1,1530)	1:317:A:TYR:HB3	1:388:A:GLU:H	7	0.12
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD2	20	0.12
(1,1521)	1:316:A:ASN:H	1:349:A:ARG:HD3	20	0.12
(1,1485)	1:314:A:MET:HB2	1:319:A:ARG:H	18	0.12
(1,1485)	1:314:A:MET:HB3	1:319:A:ARG:H	18	0.12
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	11	0.12
(1,1451)	1:313:A:PHE:HZ	1:345:A:THR:HA	12	0.12
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:HA	14	0.12
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:HA	14	0.12
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:HA	14	0.12
(1,1352)	1:305:A:PHE:HE1	1:307:A:MET:HA	14	0.12
(1,1352)	1:305:A:PHE:HE2	1:307:A:MET:HA	14	0.12
(1,1348)	1:305:A:PHE:HZ	1:308:A:ASP:HA	9	0.12
(1,1320)	1:302:A:GLN:HA	1:328:A:SER:HA	16	0.12
(1,1254)	1:300:A:TYR:HA	1:306:A:ILE:HB	5	0.12
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	2	0.12
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	2	0.12
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	7	0.12
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	7	0.12
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	19	0.12
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	10	0.12
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	10	0.12
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	10	0.12
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	10	0.12
(1,1199)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	10	0.12
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	10	0.12
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	10	0.12
(1,1199)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	10	0.12
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD11	3	0.12
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD12	3	0.12
(1,1198)	1:299:A:LEU:HA	1:325:A:ILE:HD13	3	0.12
(1,1171)	1:298:A:LYS:HA	1:307:A:MET:H	4	0.12
(1,1156)	1:298:A:LYS:HG2	1:323:A:GLY:H	15	0.12
(1,1156)	1:298:A:LYS:HG3	1:323:A:GLY:H	15	0.12
(1,1071)	1:295:A:HIS:HE1	1:311:A:GLU:HA	16	0.12
(1,1052)	1:293:A:HIS:HB2	1:295:A:HIS:H	7	0.12
(1,1052)	1:293:A:HIS:HB3	1:295:A:HIS:H	7	0.12
(1,1043)	1:291:A:ARG:HA	1:293:A:HIS:HA	11	0.12
(1,1036)	1:290:A:ASN:HB2	1:292:A:ASP:H	12	0.12
(1,1036)	1:290:A:ASN:HB3	1:292:A:ASP:H	12	0.12
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	9	0.12
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	2	0.12
(1,877)	1:280:A:ILE:HA	1:322:A:ARG:H	12	0.12
(1,780)	1:277:A:LEU:H	1:325:A:ILE:HB	2	0.12
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	1	0.12
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	1	0.12
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	13	0.12
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	13	0.12
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	16	0.12
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	16	0.12
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	14	0.12
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	5	0.12
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	8	0.12
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	11	0.12
(1,573)	1:264:A:SER:HB2	1:359:A:MET:HE1	20	0.12
(1,573)	1:264:A:SER:HB2	1:359:A:MET:HE2	20	0.12
(1,573)	1:264:A:SER:HB2	1:359:A:MET:HE3	20	0.12
(1,573)	1:264:A:SER:HB3	1:359:A:MET:HE1	20	0.12
(1,573)	1:264:A:SER:HB3	1:359:A:MET:HE2	20	0.12
(1,573)	1:264:A:SER:HB3	1:359:A:MET:HE3	20	0.12
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	11	0.12
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	12	0.12
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	20	0.12
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	6	0.12
(1,381)	1:251:A:LYS:HA	1:255:A:HIS:H	13	0.12
(1,381)	1:251:A:LYS:HA	1:255:A:HIS:H	16	0.12
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	11	0.12
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	11	0.12
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	11	0.12
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	11	0.12
(1,332)	1:250:A:TYR:HE2	1:322:A:ARG:HB2	2	0.12
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	13	0.12
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	1	0.12
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	8	0.12
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	16	0.12
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	14	0.12
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	14	0.12
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	20	0.12
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	20	0.12
(1,36)	1:233:A:LEU:HD21	1:265:A:HIS:HB2	19	0.12
(1,36)	1:233:A:LEU:HD21	1:265:A:HIS:HB3	19	0.12
(1,36)	1:233:A:LEU:HD22	1:265:A:HIS:HB2	19	0.12
(1,36)	1:233:A:LEU:HD22	1:265:A:HIS:HB3	19	0.12
(1,36)	1:233:A:LEU:HD23	1:265:A:HIS:HB2	19	0.12
(1,36)	1:233:A:LEU:HD23	1:265:A:HIS:HB3	19	0.12
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD21	16	0.11
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD22	16	0.11
(1,3663)	1:395:A:ALA:HB1	2:630:B:LEU:HD23	16	0.11
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD21	16	0.11
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD22	16	0.11
(1,3663)	1:395:A:ALA:HB2	2:630:B:LEU:HD23	16	0.11
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD21	16	0.11
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD22	16	0.11
(1,3663)	1:395:A:ALA:HB3	2:630:B:LEU:HD23	16	0.11
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD11	16	0.11
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD12	16	0.11
(1,3658)	1:405:A:THR:HG21	2:607:B:ILE:HD13	16	0.11
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD11	16	0.11
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD12	16	0.11
(1,3658)	1:405:A:THR:HG22	2:607:B:ILE:HD13	16	0.11
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD11	16	0.11
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD12	16	0.11
(1,3658)	1:405:A:THR:HG23	2:607:B:ILE:HD13	16	0.11
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG21	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG22	9	0.11
(1,3657)	1:455:A:ILE:HD11	2:605:B:THR:HG23	9	0.11
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG21	9	0.11
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG22	9	0.11
(1,3657)	1:455:A:ILE:HD12	2:605:B:THR:HG23	9	0.11
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG21	9	0.11
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG22	9	0.11
(1,3657)	1:455:A:ILE:HD13	2:605:B:THR:HG23	9	0.11
(1,3558)	1:471:A:TYR:HA	1:473:A:THR:H	9	0.11
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD21	1	0.11
(1,3519)	1:467:A:TRP:HA	1:470:A:ASN:HD22	1	0.11
(1,3505)	1:465:A:ASP:HB2	1:466:A:GLU:H	2	0.11
(1,3505)	1:465:A:ASP:HB3	1:466:A:GLU:H	2	0.11
(1,3467)	1:462:A:ASP:H	1:464:A:ILE:H	17	0.11
(1,3400)	1:451:A:ARG:HA	1:455:A:ILE:H	5	0.11
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	10	0.11
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	10	0.11
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	10	0.11
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	10	0.11
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB2	16	0.11
(1,3351)	1:447:A:LEU:HB2	1:451:A:ARG:HB3	16	0.11
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB2	16	0.11
(1,3351)	1:447:A:LEU:HB3	1:451:A:ARG:HB3	16	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	4	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	4	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	4	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG21	10	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG22	10	0.11
(1,3346)	1:447:A:LEU:HA	1:457:A:VAL:HG23	10	0.11
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG2	16	0.11
(1,3328)	1:445:A:PRO:HA	1:448:A:GLU:HG3	16	0.11
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	9	0.11
(1,3214)	1:435:A:ALA:HB1	1:441:A:ALA:HA	13	0.11
(1,3214)	1:435:A:ALA:HB2	1:441:A:ALA:HA	13	0.11
(1,3214)	1:435:A:ALA:HB3	1:441:A:ALA:HA	13	0.11
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB2	1	0.11
(1,3196)	1:434:A:THR:H	1:482:A:SER:HB3	1	0.11
(1,3161)	1:432:A:TYR:HA	1:460:A:LEU:H	18	0.11
(1,3160)	1:432:A:TYR:H	1:481:A:GLN:H	10	0.11
(1,3147)	1:431:A:TYR:H	1:458:A:LEU:HG	10	0.11
(1,3142)	1:431:A:TYR:HA	1:480:A:PHE:HA	14	0.11
(1,3137)	1:431:A:TYR:HB2	1:482:A:SER:HA	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3137)	1:431:A:TYR:HB3	1:482:A:SER:HA	11	0.11
(1,3136)	1:431:A:TYR:HA	1:482:A:SER:HA	3	0.11
(1,3111)	1:430:A:ILE:H	1:481:A:GLN:H	7	0.11
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	18	0.11
(1,3105)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	18	0.11
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	18	0.11
(1,3105)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	18	0.11
(1,3095)	1:429:A:LYS:HA	1:480:A:PHE:HA	9	0.11
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	19	0.11
(1,3091)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	19	0.11
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	19	0.11
(1,3091)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	19	0.11
(1,3069)	1:427:A:GLN:HE21	1:455:A:ILE:HA	1	0.11
(1,3069)	1:427:A:GLN:HE22	1:455:A:ILE:HA	1	0.11
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE21	19	0.11
(1,3048)	1:424:A:LYS:H	1:427:A:GLN:HE22	19	0.11
(1,3030)	1:423:A:MET:HE1	1:428:A:GLU:H	2	0.11
(1,3030)	1:423:A:MET:HE2	1:428:A:GLU:H	2	0.11
(1,3030)	1:423:A:MET:HE3	1:428:A:GLU:H	2	0.11
(1,2939)	1:417:A:GLU:HA	1:420:A:VAL:HB	2	0.11
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE1	8	0.11
(1,2860)	1:410:A:SER:HA	1:438:A:TYR:HE2	8	0.11
(1,2836)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	18	0.11
(1,2730)	1:403:A:ALA:H	1:458:A:LEU:HA	6	0.11
(1,2712)	1:402:A:PHE:H	1:413:A:THR:H	19	0.11
(1,2697)	1:402:A:PHE:HD1	1:461:A:SER:H	7	0.11
(1,2697)	1:402:A:PHE:HD2	1:461:A:SER:H	7	0.11
(1,2639)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	13	0.11
(1,2639)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	13	0.11
(1,2598)	1:395:A:ALA:HA	1:399:A:LEU:H	17	0.11
(1,2576)	1:393:A:GLN:HA	1:396:A:ILE:HB	17	0.11
(1,2574)	1:393:A:GLN:H	1:396:A:ILE:H	18	0.11
(1,2453)	1:384:A:GLU:HA	1:467:A:TRP:HZ3	1	0.11
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	19	0.11
(1,2323)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	19	0.11
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	19	0.11
(1,2323)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	19	0.11
(1,2294)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	10	0.11
(1,2281)	1:375:A:TRP:HD1	1:412:A:GLN:HE21	5	0.11
(1,2281)	1:375:A:TRP:HD1	1:412:A:GLN:HE22	5	0.11
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	8	0.11
(1,2231)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	8	0.11
(1,2231)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	8	0.11
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD1	5	0.11
(1,2122)	1:364:A:ALA:HA	1:371:A:TYR:HD2	5	0.11
(1,2063)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	17	0.11
(1,2048)	1:360:A:LEU:HA	1:364:A:ALA:H	20	0.11
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB2	10	0.11
(1,1971)	1:355:A:ARG:H	1:357:A:LEU:HB3	10	0.11
(1,1892)	1:349:A:ARG:HG2	1:353:A:THR:H	14	0.11
(1,1892)	1:349:A:ARG:HG3	1:353:A:THR:H	14	0.11
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	2	0.11
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	2	0.11
(1,1813)	1:342:A:SER:HB2	1:343:A:THR:H	19	0.11
(1,1813)	1:342:A:SER:HB3	1:343:A:THR:H	19	0.11
(1,1762)	1:337:A:GLU:HA	1:340:A:GLN:H	15	0.11
(1,1696)	1:331:A:PRO:HB2	1:338:A:ILE:HB	20	0.11
(1,1696)	1:331:A:PRO:HB3	1:338:A:ILE:HB	20	0.11
(1,1580)	1:319:A:ARG:HA	1:321:A:VAL:HB	3	0.11
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD21	2	0.11
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD22	2	0.11
(1,1551)	1:318:A:LEU:HD21	1:382:A:LEU:HD23	2	0.11
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD21	2	0.11
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD22	2	0.11
(1,1551)	1:318:A:LEU:HD22	1:382:A:LEU:HD23	2	0.11
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD21	2	0.11
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD22	2	0.11
(1,1551)	1:318:A:LEU:HD23	1:382:A:LEU:HD23	2	0.11
(1,1533)	1:317:A:TYR:HB2	1:385:A:GLY:H	11	0.11
(1,1533)	1:317:A:TYR:HB3	1:385:A:GLY:H	11	0.11
(1,1503)	1:315:A:PRO:HD2	1:350:A:ASN:HA	5	0.11
(1,1503)	1:315:A:PRO:HD3	1:350:A:ASN:HA	5	0.11
(1,1382)	1:308:A:ASP:HA	1:310:A:ALA:H	3	0.11
(1,1381)	1:307:A:MET:HB2	1:308:A:ASP:H	9	0.11
(1,1381)	1:307:A:MET:HB3	1:308:A:ASP:H	9	0.11
(1,1381)	1:307:A:MET:HB2	1:308:A:ASP:H	20	0.11
(1,1381)	1:307:A:MET:HB3	1:308:A:ASP:H	20	0.11
(1,1333)	1:303:A:ARG:H	1:327:A:SER:H	19	0.11
(1,1323)	1:302:A:GLN:H	1:327:A:SER:H	11	0.11
(1,1317)	1:302:A:GLN:H	1:329:A:ASP:H	1	0.11
(1,1254)	1:300:A:TYR:HA	1:306:A:ILE:HB	11	0.11
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE1	8	0.11
(1,1248)	1:300:A:TYR:H	1:313:A:PHE:HE2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:300:A:TYR:H	1:327:A:SER:H	7	0.11
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	10	0.11
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	13	0.11
(1,1218)	1:299:A:LEU:H	1:306:A:ILE:H	15	0.11
(1,1196)	1:299:A:LEU:HA	1:325:A:ILE:H	13	0.11
(1,1131)	1:297:A:LEU:H	1:310:A:ALA:H	16	0.11
(1,1089)	1:296:A:GLY:H	1:311:A:GLU:HA	18	0.11
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	3	0.11
(1,1068)	1:295:A:HIS:HE1	1:316:A:ASN:HA	3	0.11
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	3	0.11
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	3	0.11
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	17	0.11
(1,869)	1:280:A:ILE:HD11	1:360:A:LEU:HA	2	0.11
(1,869)	1:280:A:ILE:HD12	1:360:A:LEU:HA	2	0.11
(1,869)	1:280:A:ILE:HD13	1:360:A:LEU:HA	2	0.11
(1,740)	1:275:A:THR:H	1:328:A:SER:H	16	0.11
(1,652)	1:268:A:VAL:H	1:273:A:GLU:HA	2	0.11
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	3	0.11
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	13	0.11
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	13	0.11
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB2	12	0.11
(1,524)	1:262:A:THR:HG21	1:370:A:LYS:HB3	12	0.11
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB2	12	0.11
(1,524)	1:262:A:THR:HG22	1:370:A:LYS:HB3	12	0.11
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB2	12	0.11
(1,524)	1:262:A:THR:HG23	1:370:A:LYS:HB3	12	0.11
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	6	0.11
(1,510)	1:261:A:LEU:H	1:282:A:SER:HA	7	0.11
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	2	0.11
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	5	0.11
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	16	0.11
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	13	0.11
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	13	0.11
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	13	0.11
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	13	0.11
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	10	0.11
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	10	0.11
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	6	0.11
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA2	2	0.11
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA3	2	0.11
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA2	2	0.11
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	5	0.11
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	5	0.11
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	6	0.11
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	10	0.11
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	9	0.11
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	16	0.11
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	7	0.11
(1,150)	1:238:A:LYS:HG2	1:265:A:HIS:HE1	6	0.11
(1,150)	1:238:A:LYS:HG3	1:265:A:HIS:HE1	6	0.11
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	5	0.11
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	5	0.11
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	18	0.11
(1,66)	1:234:A:TRP:HZ2	1:304:A:VAL:H	13	0.11
(1,44)	1:233:A:LEU:HD11	1:242:A:THR:H	8	0.11
(1,44)	1:233:A:LEU:HD12	1:242:A:THR:H	8	0.11
(1,44)	1:233:A:LEU:HD13	1:242:A:THR:H	8	0.11
(1,3586)	1:474:A:GLU:HA	1:479:A:PRO:HA	18	0.1
(1,3574)	1:473:A:THR:HA	1:480:A:PHE:H	15	0.1
(1,3570)	1:472:A:LEU:HD21	1:474:A:GLU:HA	6	0.1
(1,3570)	1:472:A:LEU:HD22	1:474:A:GLU:HA	6	0.1
(1,3570)	1:472:A:LEU:HD23	1:474:A:GLU:HA	6	0.1
(1,3521)	1:467:A:TRP:HA	1:469:A:MET:H	7	0.1
(1,3508)	1:466:A:GLU:HA	1:469:A:MET:H	10	0.1
(1,3464)	1:462:A:ASP:H	1:465:A:ASP:H	6	0.1
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	19	0.1
(1,3441)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	19	0.1
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	19	0.1
(1,3441)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	19	0.1
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	19	0.1
(1,3441)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	19	0.1
(1,3345)	1:447:A:LEU:HD21	1:457:A:VAL:HG11	1	0.1
(1,3345)	1:447:A:LEU:HD21	1:457:A:VAL:HG12	1	0.1
(1,3345)	1:447:A:LEU:HD21	1:457:A:VAL:HG13	1	0.1
(1,3345)	1:447:A:LEU:HD22	1:457:A:VAL:HG11	1	0.1
(1,3345)	1:447:A:LEU:HD22	1:457:A:VAL:HG12	1	0.1
(1,3345)	1:447:A:LEU:HD22	1:457:A:VAL:HG13	1	0.1
(1,3345)	1:447:A:LEU:HD23	1:457:A:VAL:HG11	1	0.1
(1,3345)	1:447:A:LEU:HD23	1:457:A:VAL:HG12	1	0.1
(1,3345)	1:447:A:LEU:HD23	1:457:A:VAL:HG13	1	0.1
(1,3317)	1:444:A:SER:H	1:447:A:LEU:H	7	0.1
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD21	14	0.1
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD22	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3300)	1:442:A:LYS:HA	1:459:A:LEU:HD23	14	0.1
(1,3229)	1:437:A:SER:H	1:441:A:ALA:H	16	0.1
(1,3198)	1:434:A:THR:HG21	1:466:A:GLU:HA	16	0.1
(1,3198)	1:434:A:THR:HG22	1:466:A:GLU:HA	16	0.1
(1,3198)	1:434:A:THR:HG23	1:466:A:GLU:HA	16	0.1
(1,3152)	1:431:A:TYR:HB2	1:456:A:GLU:H	5	0.1
(1,3152)	1:431:A:TYR:HB3	1:456:A:GLU:H	5	0.1
(1,3075)	1:427:A:GLN:HG2	1:429:A:LYS:H	12	0.1
(1,3075)	1:427:A:GLN:HG3	1:429:A:LYS:H	12	0.1
(1,3046)	1:424:A:LYS:H	1:427:A:GLN:H	20	0.1
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG2	11	0.1
(1,3036)	1:423:A:MET:HE1	1:427:A:GLN:HG3	11	0.1
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG2	11	0.1
(1,3036)	1:423:A:MET:HE2	1:427:A:GLN:HG3	11	0.1
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG2	11	0.1
(1,3036)	1:423:A:MET:HE3	1:427:A:GLN:HG3	11	0.1
(1,2938)	1:417:A:GLU:HA	1:420:A:VAL:H	1	0.1
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB2	18	0.1
(1,2936)	1:417:A:GLU:HA	1:421:A:SER:HB3	18	0.1
(1,2935)	1:417:A:GLU:HB2	1:421:A:SER:H	11	0.1
(1,2935)	1:417:A:GLU:HB3	1:421:A:SER:H	11	0.1
(1,2861)	1:410:A:SER:HA	1:438:A:TYR:HD2	18	0.1
(1,2808)	1:405:A:THR:HA	1:408:A:ASP:HA	17	0.1
(1,2770)	1:404:A:SER:H	1:414:A:VAL:HB	17	0.1
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG11	17	0.1
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG12	17	0.1
(1,2737)	1:403:A:ALA:HA	1:414:A:VAL:HG13	17	0.1
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG11	12	0.1
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG12	12	0.1
(1,2736)	1:403:A:ALA:H	1:414:A:VAL:HG13	12	0.1
(1,2734)	1:403:A:ALA:HA	1:414:A:VAL:H	13	0.1
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	2	0.1
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	2	0.1
(1,2690)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	2	0.1
(1,2518)	1:387:A:ALA:HB1	1:467:A:TRP:HH2	12	0.1
(1,2518)	1:387:A:ALA:HB2	1:467:A:TRP:HH2	12	0.1
(1,2518)	1:387:A:ALA:HB3	1:467:A:TRP:HH2	12	0.1
(1,2434)	1:383:A:LYS:HE2	1:402:A:PHE:HE2	4	0.1
(1,2294)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	17	0.1
(1,2285)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	11	0.1
(1,2143)	1:365:A:LYS:H	1:367:A:ASP:H	16	0.1
(1,2064)	1:361:A:GLU:HA	1:399:A:LEU:HA	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB2	9	0.1
(1,2010)	1:358:A:GLN:HA	1:361:A:GLU:HB3	9	0.1
(1,2005)	1:357:A:LEU:HB2	1:358:A:GLN:H	5	0.1
(1,2005)	1:357:A:LEU:HB3	1:358:A:GLN:H	5	0.1
(1,1999)	1:357:A:LEU:HA	1:360:A:LEU:HD11	4	0.1
(1,1999)	1:357:A:LEU:HA	1:360:A:LEU:HD12	4	0.1
(1,1999)	1:357:A:LEU:HA	1:360:A:LEU:HD13	4	0.1
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	7	0.1
(1,1913)	1:351:A:ALA:HA	1:355:A:ARG:H	10	0.1
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD21	11	0.1
(1,1872)	1:347:A:ASN:HA	1:350:A:ASN:HD22	11	0.1
(1,1852)	1:345:A:THR:HB	1:346:A:ARG:H	11	0.1
(1,1852)	1:345:A:THR:HB	1:346:A:ARG:H	19	0.1
(1,1841)	1:345:A:THR:HA	1:349:A:ARG:H	16	0.1
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG2	5	0.1
(1,1608)	1:320:A:PHE:HA	1:322:A:ARG:HG3	5	0.1
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE1	1	0.1
(1,1599)	1:320:A:PHE:HZ	1:374:A:PHE:HE2	1	0.1
(1,1222)	1:299:A:LEU:H	1:305:A:PHE:HA	10	0.1
(1,1073)	1:295:A:HIS:HA	1:309:A:ASP:HA	20	0.1
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD2	13	0.1
(1,1057)	1:294:A:LYS:H	1:319:A:ARG:HD3	13	0.1
(1,1022)	1:289:A:TRP:HZ2	1:381:A:VAL:H	10	0.1
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	16	0.1
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	2	0.1
(1,970)	1:285:A:PRO:HG2	1:287:A:ASP:H	5	0.1
(1,970)	1:285:A:PRO:HG3	1:287:A:ASP:H	5	0.1
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	14	0.1
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	14	0.1
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	14	0.1
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	14	0.1
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	14	0.1
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	14	0.1
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	14	0.1
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	14	0.1
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	9	0.1
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	5	0.1
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	18	0.1
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	2	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE1	1	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE2	1	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE3	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE1	18	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE2	18	0.1
(1,548)	1:263:A:TRP:HA	1:359:A:MET:HE3	18	0.1
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	15	0.1
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	10	0.1
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	2	0.1
(1,92)	1:234:A:TRP:HZ3	1:249:A:PHE:HZ	7	0.1
(1,88)	1:234:A:TRP:HB2	1:265:A:HIS:HD2	7	0.1
(1,88)	1:234:A:TRP:HB3	1:265:A:HIS:HD2	7	0.1
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD2	2	0.1
(1,6)	1:231:A:GLN:HB2	1:236:A:ARG:HD3	2	0.1
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD2	2	0.1
(1,6)	1:231:A:GLN:HB3	1:236:A:ARG:HD3	2	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found