



Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 19459
Title : CR1 Sushi domains 1 and 2
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Deposited on : 2013-08-27

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

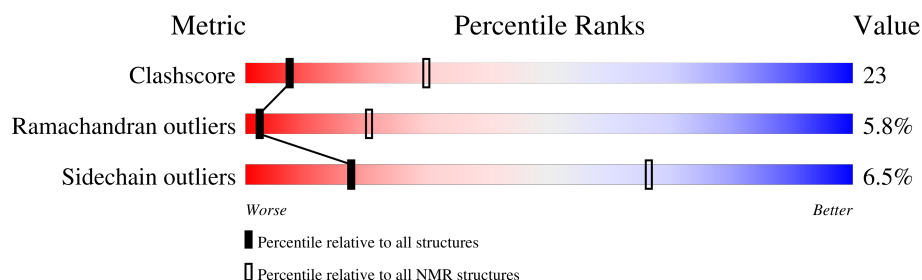
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	128	52% 40% • 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:122 (122)	1.36	13

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1897 atoms, of which 934 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Complement receptor type 1.

Mol	Chain	Residues	Atoms						Trace
1	A	122	Total	C	H	N	O	S	0
			1897	607	934	170	177	9	

There are 7 discrepancies between the modelled and reference sequences:

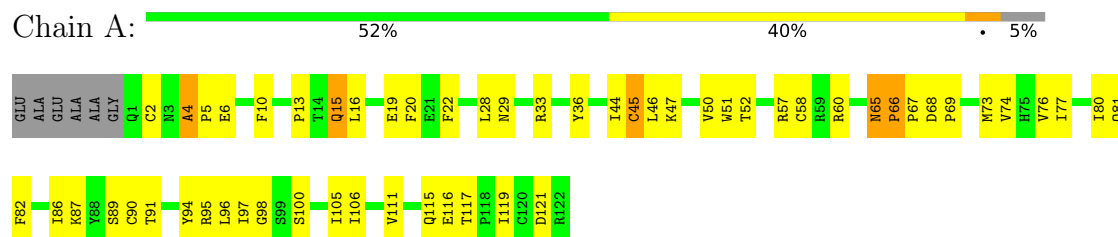
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLU	-	expression tag	UNP P17927
A	-4	ALA	-	expression tag	UNP P17927
A	-3	GLU	-	expression tag	UNP P17927
A	-2	ALA	-	expression tag	UNP P17927
A	-1	ALA	-	expression tag	UNP P17927
A	15	GLN	ASN	conflict	UNP P17927
A	115	GLN	ASN	conflict	UNP P17927

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: Complement receptor type 1

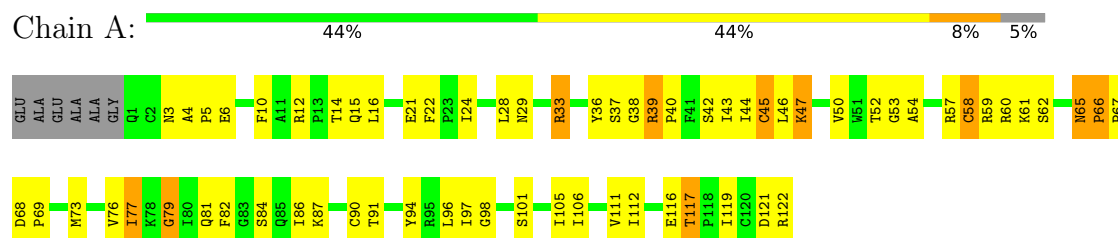


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

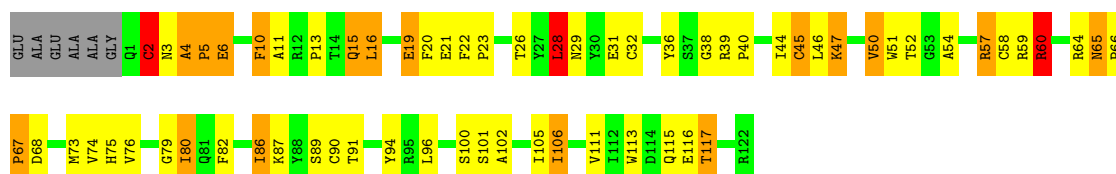
- Molecule 1: Complement receptor type 1



4.2.2 Score per residue for model 2

- Molecule 1: Complement receptor type 1

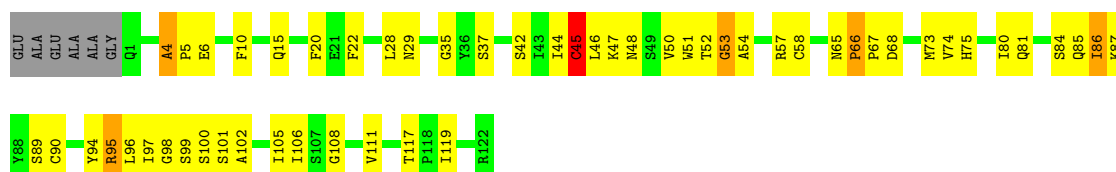




4.2.3 Score per residue for model 3

- Molecule 1: Complement receptor type 1

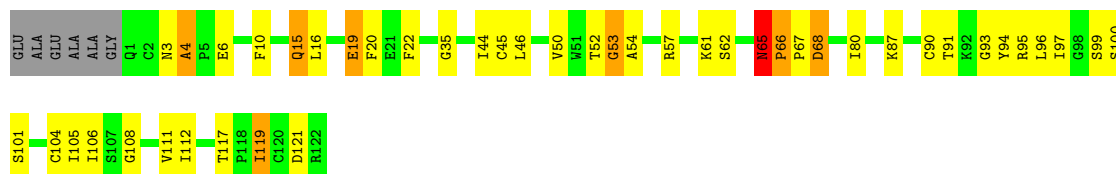
Chain A: 53% 38% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Complement receptor type 1

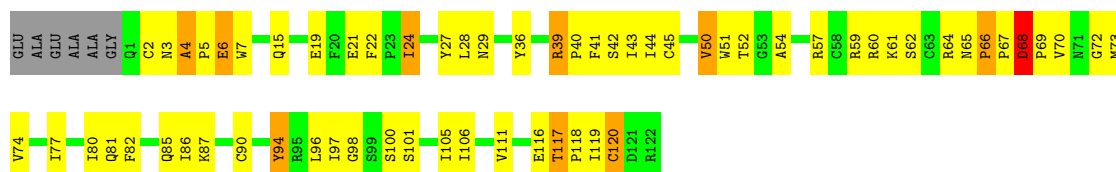
Chain A: 60% 29% 5%



4.2.5 Score per residue for model 5

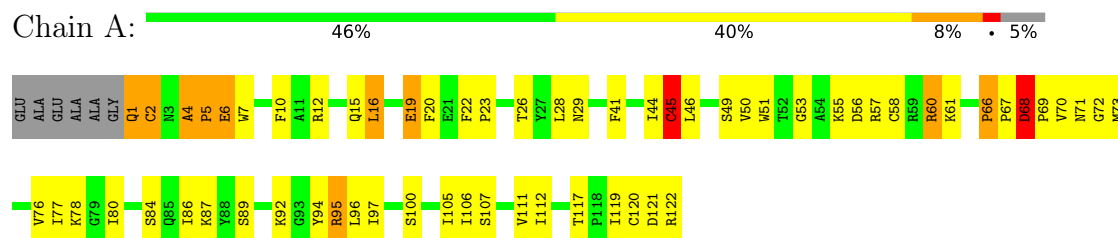
- Molecule 1: Complement receptor type 1

Chain A: 46% 41% 7%



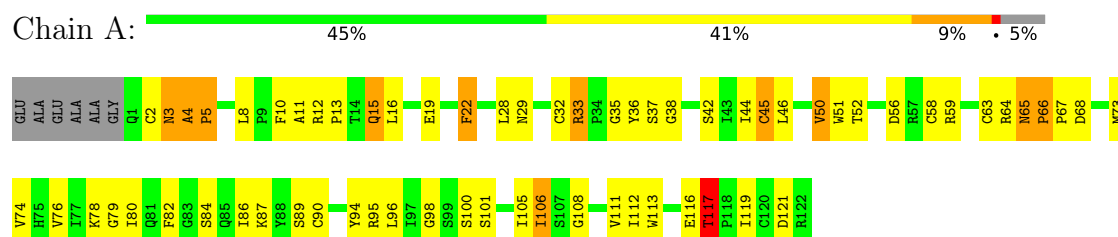
4.2.6 Score per residue for model 6

- Molecule 1: Complement receptor type 1



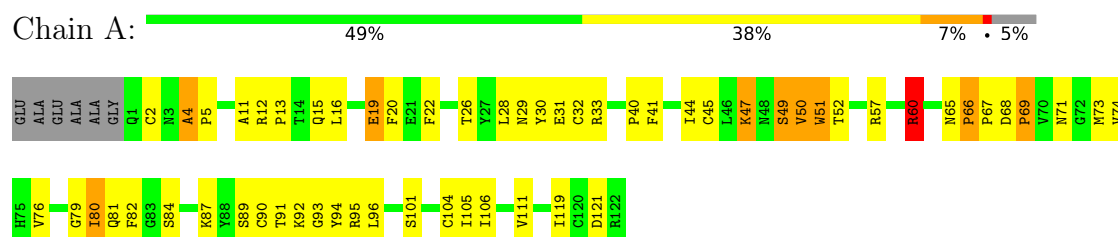
4.2.7 Score per residue for model 7

- Molecule 1: Complement receptor type 1



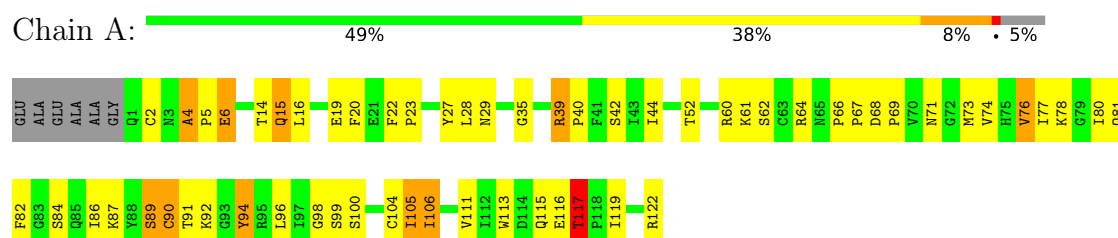
4.2.8 Score per residue for model 8

- Molecule 1: Complement receptor type 1



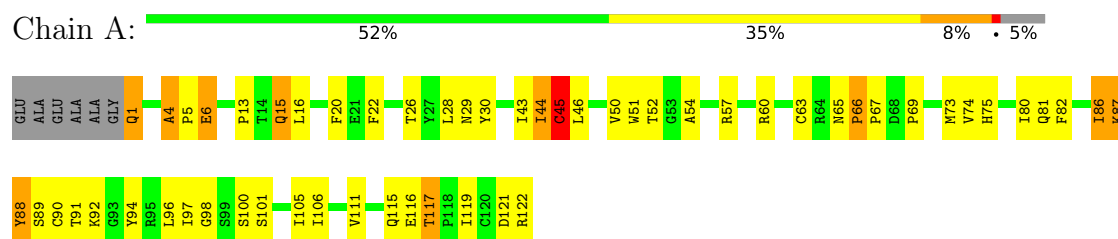
4.2.9 Score per residue for model 9

- Molecule 1: Complement receptor type 1



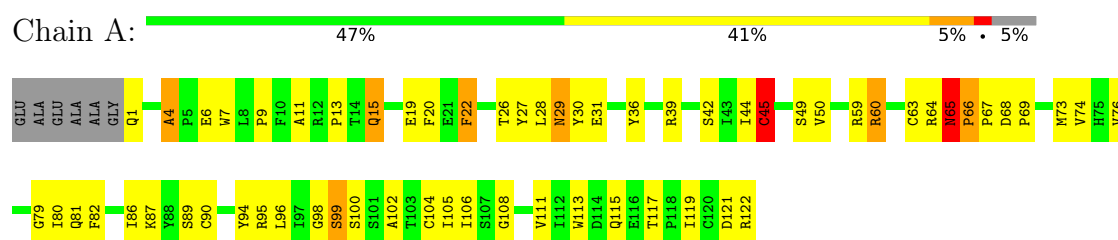
4.2.10 Score per residue for model 10

- Molecule 1: Complement receptor type 1



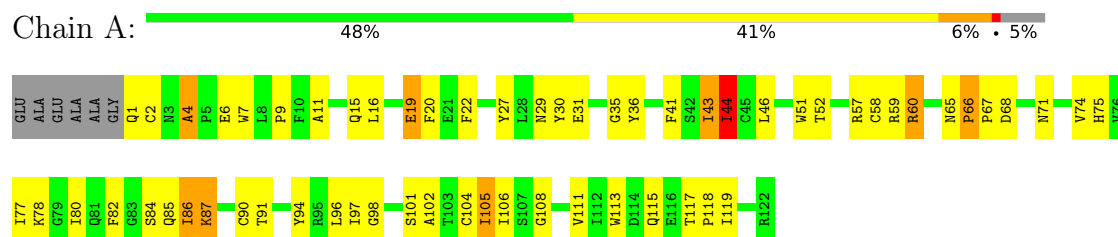
4.2.11 Score per residue for model 11

- Molecule 1: Complement receptor type 1



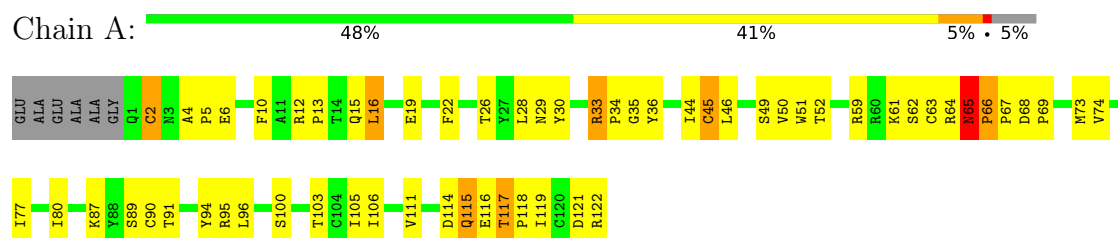
4.2.12 Score per residue for model 12

- Molecule 1: Complement receptor type 1



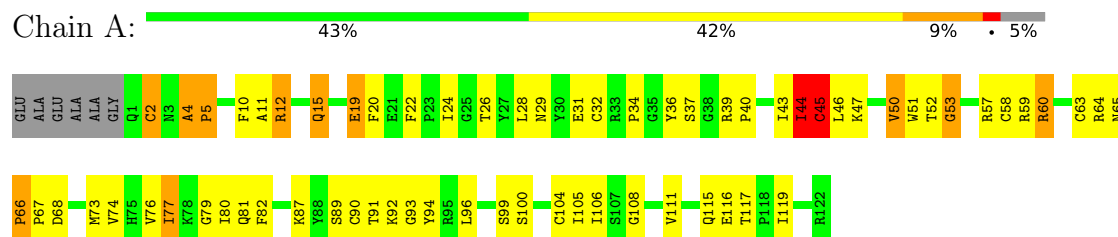
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Complement receptor type 1



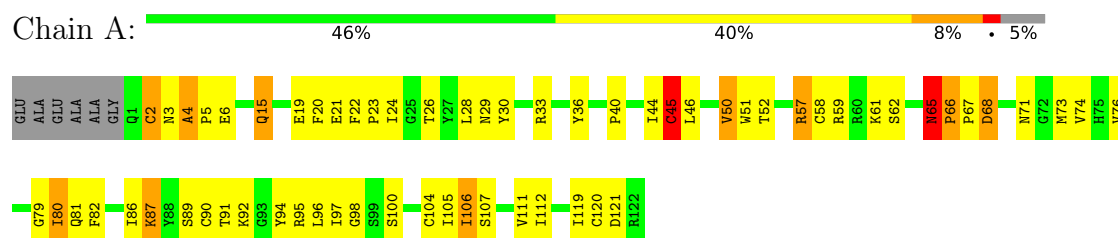
4.2.14 Score per residue for model 14

- Molecule 1: Complement receptor type 1



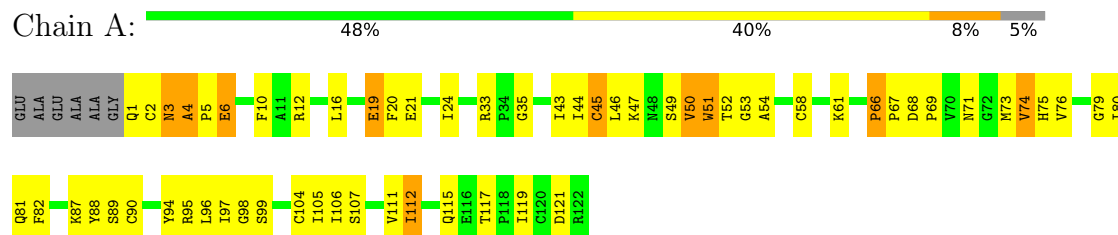
4.2.15 Score per residue for model 15

- Molecule 1: Complement receptor type 1



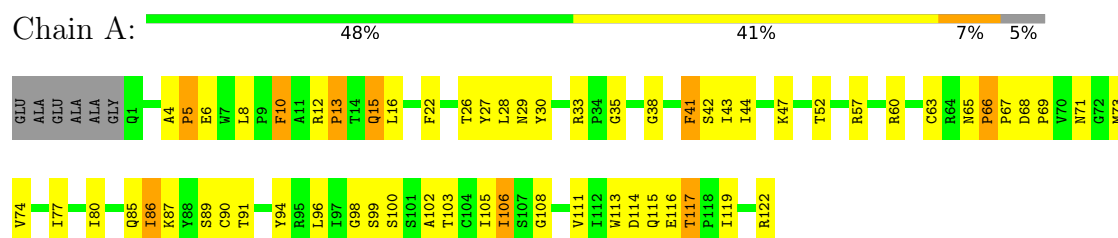
4.2.16 Score per residue for model 16

- Molecule 1: Complement receptor type 1



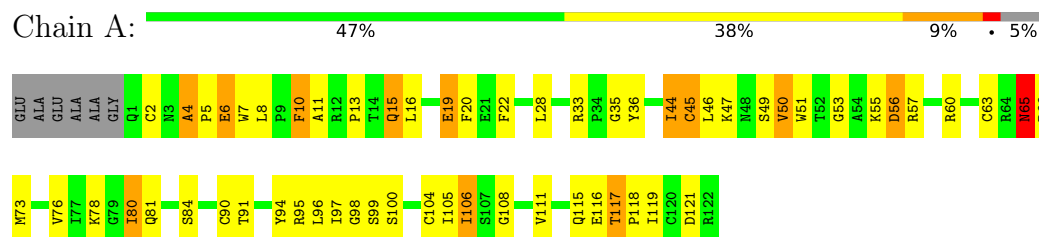
4.2.17 Score per residue for model 17

- Molecule 1: Complement receptor type 1



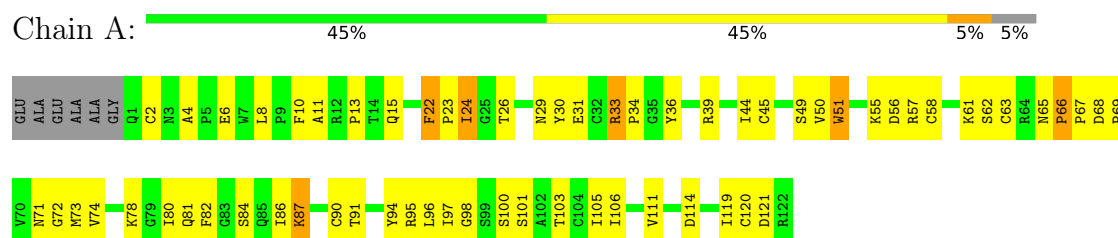
4.2.18 Score per residue for model 18

- Molecule 1: Complement receptor type 1



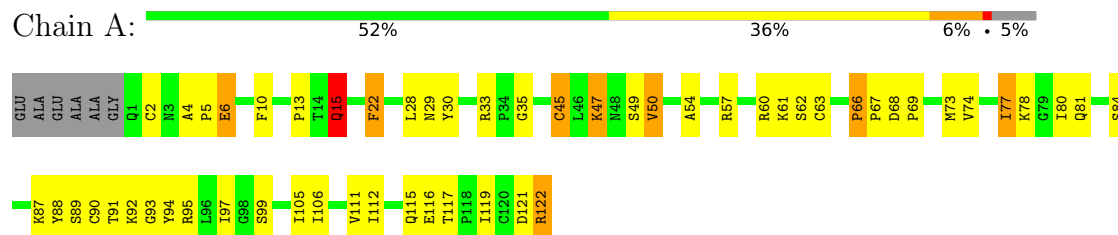
4.2.19 Score per residue for model 19

- Molecule 1: Complement receptor type 1



4.2.20 Score per residue for model 20

- Molecule 1: Complement receptor type 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1370
Number of shifts mapped to atoms	1365
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.20±0.06	4±1/989 (0.4± 0.1%)	1.13±0.05	3±2/1342 (0.2± 0.2%)
All	All	1.21	78/19780 (0.4%)	1.13	61/26840 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.7
All	All	0	14

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
1	A	66	PRO	C-N	10.92	1.42	1.33	16	9
1	A	66	PRO	CA-C	10.22	1.61	1.52	16	15
1	A	90	CYS	N-CA	-8.29	1.40	1.46	9	1
1	A	47	LYS	CA-C	-8.24	1.42	1.52	1	2
1	A	79	GLY	C-N	-8.06	1.24	1.33	1	1
1	A	19	GLU	C-N	-7.35	1.24	1.33	9	11
1	A	89	SER	C-N	-7.28	1.26	1.33	9	1
1	A	90	CYS	C-N	-6.93	1.24	1.33	9	1
1	A	45	CYS	N-CA	6.83	1.55	1.46	6	5
1	A	15	GLN	C-N	-6.71	1.25	1.33	20	1
1	A	119	ILE	C-O	-6.50	1.17	1.24	4	1
1	A	65	ASN	C-N	6.50	1.41	1.33	13	4
1	A	79	GLY	N-CA	-6.43	1.39	1.45	1	1
1	A	88	TYR	N-CA	-6.30	1.38	1.46	20	2
1	A	87	LYS	CA-C	-6.19	1.45	1.52	10	1
1	A	50	VAL	C-N	-5.99	1.25	1.33	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	LYS	N-CA	-5.97	1.38	1.46	9	2
1	A	7	TRP	N-CA	-5.96	1.38	1.46	5	1
1	A	50	VAL	C-O	-5.80	1.17	1.23	16	2
1	A	16	LEU	C-N	-5.79	1.26	1.34	7	3
1	A	69	PRO	N-CA	-5.77	1.40	1.46	8	1
1	A	45	CYS	CA-C	5.65	1.60	1.52	14	1
1	A	13	PRO	C-N	-5.62	1.26	1.34	17	1
1	A	28	LEU	CA-C	-5.43	1.46	1.52	2	1
1	A	3	ASN	CA-C	-5.36	1.46	1.53	7	1
1	A	120	CYS	C-N	5.32	1.40	1.33	5	1
1	A	92	LYS	C-N	-5.29	1.26	1.33	9	2
1	A	29	ASN	N-CA	-5.18	1.40	1.46	11	1
1	A	47	LYS	C-N	-5.16	1.27	1.33	20	1
1	A	87	LYS	C-N	-5.15	1.26	1.33	10	1
1	A	44	ILE	CA-C	5.07	1.58	1.52	14	1
1	A	5	PRO	C-N	-5.01	1.26	1.33	8	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	CYS	CA-C-O	8.20	122.70	117.94	9	1
1	A	77	ILE	CB-CA-C	-6.72	103.37	111.97	1	2
1	A	15	GLN	CA-C-N	6.48	128.96	120.28	20	1
1	A	15	GLN	C-N-CA	6.48	128.96	120.28	20	1
1	A	59	ARG	CA-C-N	6.47	130.06	120.87	12	2
1	A	59	ARG	C-N-CA	6.47	130.06	120.87	12	2
1	A	106	ILE	CB-CA-C	-6.34	103.29	110.96	7	6
1	A	2	CYS	N-CA-CB	6.28	119.78	110.49	2	4
1	A	92	LYS	N-CA-C	6.20	117.84	111.14	10	1
1	A	5	PRO	CB-CA-C	-6.13	103.31	113.06	6	2
1	A	67	PRO	CB-CA-C	-5.88	102.41	112.64	2	1
1	A	22	PHE	CA-C-N	5.78	125.75	120.03	7	7
1	A	22	PHE	C-N-CA	5.78	125.75	120.03	7	7
1	A	92	LYS	CB-CA-C	-5.73	101.88	110.88	8	2
1	A	61	LYS	N-CA-C	5.62	118.88	109.95	6	1
1	A	97	ILE	N-CA-C	5.59	115.79	110.53	3	1
1	A	2	CYS	N-CA-C	-5.57	105.99	112.89	13	1
1	A	68	ASP	CA-CB-CG	5.51	118.11	112.60	18	2
1	A	10	PHE	CB-CA-C	-5.50	101.66	110.79	17	4
1	A	77	ILE	N-CA-C	5.50	116.22	110.62	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	ARG	N-CA-CB	-5.38	102.06	109.97	12	3
1	A	57	ARG	N-CA-C	5.24	117.08	111.36	2	1
1	A	95	ARG	CA-C-N	-5.21	115.83	122.77	20	2
1	A	95	ARG	C-N-CA	-5.21	115.83	122.77	20	2
1	A	58	CYS	CA-C-N	-5.21	114.29	122.73	1	1
1	A	58	CYS	C-N-CA	-5.21	114.29	122.73	1	1
1	A	10	PHE	CA-CB-CG	5.17	118.97	113.80	17	1
1	A	71	ASN	CA-CB-CG	5.01	117.61	112.60	17	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	60	ARG	Sidechain	7
1	A	122	ARG	Sidechain	4
1	A	33	ARG	Sidechain	1
1	A	64	ARG	Sidechain	1
1	A	57	ARG	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	963	934	936	45±7
All	All	19260	18680	18720	891

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PRO:HG3	1:A:74:VAL:HG23	0.95	1.38	19	6
1:A:73:MET:SD	1:A:90:CYS:HA	0.85	2.12	17	2
1:A:33:ARG:NH2	1:A:36:TYR:HB2	0.84	1.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ASN:ND2	1:A:90:CYS:HA	0.82	1.90	8	1
1:A:96:LEU:HG	1:A:119:ILE:O	0.81	1.74	16	6
1:A:5:PRO:HA	1:A:51:TRP:NE1	0.81	1.91	10	5
1:A:5:PRO:O	1:A:6:GLU:HG2	0.78	1.78	5	1
1:A:96:LEU:HD12	1:A:119:ILE:O	0.78	1.78	11	4
1:A:69:PRO:CG	1:A:74:VAL:HG23	0.78	2.09	11	5
1:A:5:PRO:HA	1:A:51:TRP:CD1	0.77	2.15	10	4
1:A:81:GLN:HG2	1:A:82:PHE:N	0.76	1.96	16	4
1:A:106:ILE:HD13	1:A:111:VAL:HG12	0.74	1.57	2	20
1:A:73:MET:HB2	1:A:89:SER:O	0.74	1.81	7	7
1:A:1:GLN:HE21	1:A:1:GLN:N	0.73	1.81	6	1
1:A:15:GLN:HB2	1:A:28:LEU:HD22	0.73	1.61	20	1
1:A:45:CYS:HA	1:A:50:VAL:O	0.72	1.84	2	8
1:A:61:LYS:HD3	1:A:62:SER:N	0.72	1.99	19	7
1:A:15:GLN:NE2	1:A:29:ASN:H	0.71	1.83	13	16
1:A:90:CYS:HB2	1:A:94:TYR:CE2	0.71	2.21	13	7
1:A:3:ASN:HA	1:A:21:GLU:OE2	0.71	1.85	16	4
1:A:32:CYS:HB3	1:A:33:ARG:NH2	0.70	2.01	7	1
1:A:32:CYS:SG	1:A:40:PRO:HG3	0.70	2.27	14	2
1:A:15:GLN:O	1:A:19:GLU:HB2	0.70	1.86	18	7
1:A:73:MET:HB3	1:A:89:SER:O	0.69	1.86	17	5
1:A:77:ILE:HD11	1:A:87:LYS:HE2	0.69	1.64	1	5
1:A:32:CYS:SG	1:A:40:PRO:HD3	0.69	2.27	2	1
1:A:8:LEU:HD21	1:A:10:PHE:CD2	0.69	2.22	18	2
1:A:35:GLY:O	1:A:106:ILE:HG13	0.68	1.88	4	1
1:A:2:CYS:HB3	1:A:50:VAL:O	0.68	1.88	6	1
1:A:23:PRO:O	1:A:24:ILE:HB	0.68	1.88	19	1
1:A:54:ALA:O	1:A:57:ARG:HG2	0.67	1.90	10	2
1:A:81:GLN:HG2	1:A:82:PHE:H	0.66	1.50	10	4
1:A:36:TYR:CG	1:A:58:CYS:HB3	0.66	2.25	15	2
1:A:37:SER:OG	1:A:59:ARG:HB2	0.66	1.91	1	3
1:A:43:ILE:HB	1:A:51:TRP:CE3	0.65	2.27	12	1
1:A:15:GLN:NE2	1:A:28:LEU:HA	0.65	2.06	11	1
1:A:2:CYS:HA	1:A:49:SER:O	0.65	1.92	8	5
1:A:28:LEU:O	1:A:42:SER:HA	0.64	1.91	7	7
1:A:61:LYS:CD	1:A:62:SER:H	0.64	2.05	15	1
1:A:15:GLN:CD	1:A:28:LEU:HB3	0.64	2.16	20	1
1:A:97:ILE:HB	1:A:119:ILE:HG21	0.64	1.70	4	11
1:A:66:PRO:N	1:A:67:PRO:HD2	0.63	2.07	2	17
1:A:90:CYS:HB2	1:A:94:TYR:CD2	0.63	2.28	17	5
1:A:46:LEU:HD12	1:A:52:THR:HG22	0.63	1.70	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ILE:O	1:A:101:SER:HA	0.63	1.92	12	6
1:A:92:LYS:HG3	1:A:93:GLY:N	0.63	2.08	20	1
1:A:4:ALA:HB2	1:A:20:PHE:HB3	0.63	1.70	16	11
1:A:24:ILE:HA	1:A:45:CYS:SG	0.63	2.34	15	2
1:A:87:LYS:HD3	1:A:101:SER:HB3	0.63	1.69	3	3
1:A:98:GLY:HA3	1:A:119:ILE:HD13	0.62	1.68	15	3
1:A:10:PHE:O	1:A:33:ARG:HG3	0.62	1.94	17	1
1:A:63:CYS:SG	1:A:113:TRP:CE2	0.62	2.92	17	1
1:A:41:PHE:HB3	1:A:57:ARG:NH2	0.62	2.10	5	2
1:A:40:PRO:HA	1:A:57:ARG:NH2	0.62	2.09	15	1
1:A:44:ILE:O	1:A:52:THR:HG23	0.62	1.93	1	9
1:A:90:CYS:SG	1:A:94:TYR:CE2	0.61	2.93	14	12
1:A:15:GLN:NE2	1:A:28:LEU:HD23	0.61	2.09	11	2
1:A:5:PRO:HB3	1:A:51:TRP:CD1	0.61	2.30	14	2
1:A:24:ILE:HG12	1:A:45:CYS:O	0.61	1.95	16	1
1:A:34:PRO:HG2	1:A:36:TYR:CE2	0.61	2.30	19	1
1:A:65:ASN:C	1:A:67:PRO:HD2	0.61	2.20	1	11
1:A:62:SER:HA	1:A:81:GLN:HG3	0.61	1.72	19	1
1:A:96:LEU:CD2	1:A:100:SER:HA	0.61	2.26	6	12
1:A:98:GLY:N	1:A:119:ILE:HD12	0.61	2.09	11	3
1:A:15:GLN:HE22	1:A:29:ASN:H	0.61	1.38	13	2
1:A:44:ILE:HD12	1:A:52:THR:HG21	0.61	1.73	12	4
1:A:65:ASN:N	1:A:66:PRO:HD3	0.60	2.11	1	4
1:A:106:ILE:CD1	1:A:111:VAL:HG12	0.60	2.26	4	8
1:A:50:VAL:O	1:A:51:TRP:CD1	0.60	2.54	8	3
1:A:99:SER:HB3	1:A:115:GLN:OE1	0.60	1.96	9	1
1:A:2:CYS:SG	1:A:51:TRP:CZ2	0.60	2.95	14	5
1:A:69:PRO:HG3	1:A:74:VAL:CG2	0.60	2.22	19	1
1:A:36:TYR:CB	1:A:58:CYS:HB3	0.60	2.25	1	3
1:A:44:ILE:H	1:A:52:THR:HG23	0.60	1.55	4	5
1:A:13:PRO:HG3	1:A:30:TYR:CD1	0.59	2.32	17	2
1:A:1:GLN:HB2	1:A:22:PHE:O	0.59	1.98	10	2
1:A:11:ALA:HA	1:A:31:GLU:O	0.59	1.98	11	6
1:A:77:ILE:HD11	1:A:87:LYS:HE3	0.59	1.75	5	4
1:A:27:TYR:CD2	1:A:44:ILE:HG12	0.58	2.32	12	2
1:A:82:PHE:CE1	1:A:106:ILE:HG12	0.58	2.32	10	7
1:A:82:PHE:HB2	1:A:111:VAL:HG11	0.58	1.74	16	2
1:A:74:VAL:HA	1:A:87:LYS:O	0.58	1.98	11	13
1:A:75:HIS:O	1:A:86:ILE:HB	0.58	1.98	12	4
1:A:90:CYS:HB2	1:A:94:TYR:CZ	0.58	2.33	13	1
1:A:43:ILE:HG21	1:A:54:ALA:HB2	0.58	1.74	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PHE:CE2	1:A:28:LEU:HD21	0.58	2.34	6	3
1:A:71:ASN:HD21	1:A:73:MET:HG3	0.58	1.59	16	1
1:A:13:PRO:HA	1:A:29:ASN:O	0.58	1.99	13	3
1:A:96:LEU:HD23	1:A:100:SER:HA	0.58	1.74	5	6
1:A:106:ILE:HD13	1:A:111:VAL:CG1	0.57	2.29	2	2
1:A:23:PRO:HG2	1:A:26:THR:OG1	0.57	1.99	6	3
1:A:81:GLN:HG3	1:A:82:PHE:N	0.57	2.15	1	3
1:A:116:GLU:O	1:A:117:THR:HB	0.57	1.99	18	11
1:A:13:PRO:HG3	1:A:30:TYR:CE1	0.57	2.33	17	1
1:A:53:GLY:O	1:A:57:ARG:HD3	0.57	1.99	14	4
1:A:68:ASP:OD1	1:A:72:GLY:HA2	0.57	1.99	6	1
1:A:35:GLY:O	1:A:106:ILE:HG21	0.57	2.00	7	2
1:A:60:ARG:CG	1:A:82:PHE:HB3	0.57	2.29	2	2
1:A:47:LYS:HB3	1:A:51:TRP:O	0.57	1.99	3	2
1:A:32:CYS:HB3	1:A:33:ARG:HH22	0.57	1.58	7	1
1:A:91:THR:O	1:A:94:TYR:CD1	0.57	2.58	10	11
1:A:71:ASN:CG	1:A:122:ARG:HH22	0.56	2.08	6	1
1:A:15:GLN:HE22	1:A:28:LEU:HA	0.56	1.60	5	4
1:A:35:GLY:HA3	1:A:106:ILE:HG21	0.56	1.77	18	2
1:A:79:GLY:O	1:A:84:SER:HB3	0.56	1.99	1	1
1:A:91:THR:HG22	1:A:93:GLY:H	0.56	1.59	20	3
1:A:1:GLN:HE21	1:A:1:GLN:H1	0.56	1.43	6	1
1:A:22:PHE:CD1	1:A:26:THR:HG21	0.56	2.36	13	3
1:A:61:LYS:HD3	1:A:62:SER:H	0.56	1.61	15	1
1:A:71:ASN:OD1	1:A:90:CYS:HB3	0.55	1.99	12	1
1:A:69:PRO:CB	1:A:73:MET:HB2	0.55	2.31	17	1
1:A:71:ASN:ND2	1:A:73:MET:SD	0.55	2.79	19	1
1:A:22:PHE:CZ	1:A:28:LEU:HD21	0.55	2.36	20	1
1:A:98:GLY:HA3	1:A:119:ILE:HD12	0.55	1.78	3	5
1:A:36:TYR:HA	1:A:59:ARG:O	0.55	2.02	5	4
1:A:65:ASN:N	1:A:66:PRO:CD	0.55	2.70	13	7
1:A:98:GLY:CA	1:A:119:ILE:HD12	0.55	2.31	9	2
1:A:76:VAL:HG23	1:A:80:ILE:HG13	0.55	1.78	2	1
1:A:15:GLN:HE22	1:A:28:LEU:CA	0.54	2.15	5	4
1:A:81:GLN:CG	1:A:82:PHE:N	0.54	2.70	16	2
1:A:60:ARG:HD3	1:A:81:GLN:NE2	0.54	2.18	14	1
1:A:96:LEU:HD21	1:A:99:SER:O	0.54	2.02	4	1
1:A:35:GLY:CA	1:A:106:ILE:HG21	0.54	2.33	18	4
1:A:11:ALA:O	1:A:12:ARG:HD2	0.54	2.02	7	1
1:A:54:ALA:HA	1:A:57:ARG:HE	0.54	1.62	2	1
1:A:107:SER:OG	1:A:112:ILE:HG12	0.54	2.03	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:TYR:OH	1:A:96:LEU:HB2	0.54	2.02	14	2
1:A:78:LYS:HB2	1:A:84:SER:OG	0.54	2.02	20	5
1:A:71:ASN:HD21	1:A:73:MET:HE3	0.53	1.62	9	1
1:A:89:SER:HA	1:A:94:TYR:OH	0.53	2.03	10	5
1:A:2:CYS:SG	1:A:22:PHE:O	0.53	2.66	12	6
1:A:11:ALA:C	1:A:13:PRO:HD3	0.53	2.29	18	2
1:A:71:ASN:HD22	1:A:90:CYS:HB3	0.53	1.63	15	1
1:A:76:VAL:HG22	1:A:79:GLY:H	0.53	1.63	8	5
1:A:60:ARG:HG3	1:A:82:PHE:HB3	0.53	1.80	14	3
1:A:90:CYS:HB3	1:A:94:TYR:CE2	0.53	2.38	18	1
1:A:71:ASN:ND2	1:A:90:CYS:HB3	0.53	2.18	15	1
1:A:76:VAL:HA	1:A:86:ILE:HG22	0.53	1.79	9	3
1:A:45:CYS:SG	1:A:51:TRP:CH2	0.53	3.02	8	2
1:A:4:ALA:HA	1:A:20:PHE:O	0.52	2.03	10	3
1:A:54:ALA:HA	1:A:57:ARG:NE	0.52	2.19	2	1
1:A:77:ILE:HD11	1:A:87:LYS:CE	0.52	2.34	1	1
1:A:106:ILE:HG22	1:A:108:GLY:H	0.52	1.64	3	4
1:A:15:GLN:CD	1:A:15:GLN:H	0.52	2.10	20	1
1:A:104:CYS:HB2	1:A:113:TRP:CE3	0.52	2.39	9	1
1:A:99:SER:HB2	1:A:115:GLN:CD	0.52	2.28	14	2
1:A:91:THR:HB	1:A:94:TYR:HB3	0.52	1.81	15	5
1:A:47:LYS:O	1:A:50:VAL:HB	0.52	2.05	1	2
1:A:16:LEU:HA	1:A:19:GLU:O	0.52	2.05	16	4
1:A:81:GLN:HG3	1:A:82:PHE:H	0.52	1.62	1	1
1:A:41:PHE:CD2	1:A:57:ARG:NH2	0.52	2.78	12	1
1:A:47:LYS:HD3	1:A:47:LYS:C	0.52	2.30	8	1
1:A:99:SER:HB2	1:A:115:GLN:OE1	0.52	2.05	14	2
1:A:82:PHE:CZ	1:A:106:ILE:HG12	0.52	2.40	8	1
1:A:95:ARG:O	1:A:121:ASP:HB3	0.52	2.05	16	3
1:A:33:ARG:HB2	1:A:34:PRO:HD2	0.51	1.80	13	1
1:A:66:PRO:N	1:A:67:PRO:CD	0.51	2.73	16	14
1:A:33:ARG:CZ	1:A:36:TYR:CD1	0.51	2.93	7	1
1:A:103:THR:HB	1:A:114:ASP:OD2	0.51	2.06	19	3
1:A:2:CYS:HA	1:A:49:SER:OG	0.51	2.05	19	1
1:A:68:ASP:OD1	1:A:69:PRO:HD2	0.51	2.05	18	2
1:A:36:TYR:HB3	1:A:58:CYS:HB3	0.51	1.82	15	4
1:A:69:PRO:CD	1:A:74:VAL:HG23	0.51	2.35	16	2
1:A:13:PRO:HG3	1:A:30:TYR:CZ	0.51	2.40	13	1
1:A:91:THR:HG21	1:A:122:ARG:HH21	0.51	1.65	20	1
1:A:78:LYS:HB2	1:A:84:SER:HA	0.51	1.81	12	1
1:A:15:GLN:HE22	1:A:29:ASN:N	0.50	2.03	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ASN:N	1:A:66:PRO:HD2	0.50	2.21	15	1
1:A:71:ASN:ND2	1:A:73:MET:HG3	0.50	2.21	16	1
1:A:44:ILE:C	1:A:46:LEU:H	0.50	2.14	18	1
1:A:4:ALA:H	1:A:21:GLU:HG2	0.50	1.65	16	2
1:A:27:TYR:CE2	1:A:44:ILE:HG12	0.50	2.41	17	4
1:A:60:ARG:HG3	1:A:82:PHE:CD2	0.50	2.41	14	1
1:A:2:CYS:HB3	1:A:51:TRP:CE2	0.50	2.42	12	1
1:A:8:LEU:HD22	1:A:57:ARG:NH2	0.50	2.22	19	1
1:A:87:LYS:CD	1:A:101:SER:HB3	0.49	2.37	3	3
1:A:68:ASP:OD2	1:A:72:GLY:HA2	0.49	2.07	5	1
1:A:70:VAL:HB	1:A:120:CYS:SG	0.49	2.48	5	2
1:A:76:VAL:HG23	1:A:76:VAL:O	0.49	2.07	15	2
1:A:82:PHE:CE1	1:A:105:ILE:HA	0.49	2.43	9	2
1:A:44:ILE:H	1:A:52:THR:CG2	0.49	2.21	17	1
1:A:119:ILE:O	1:A:120:CYS:SG	0.49	2.70	6	3
1:A:69:PRO:CG	1:A:74:VAL:HB	0.49	2.37	13	1
1:A:37:SER:O	1:A:58:CYS:HA	0.49	2.08	7	2
1:A:91:THR:HG22	1:A:93:GLY:N	0.49	2.23	4	3
1:A:73:MET:SD	1:A:90:CYS:C	0.49	2.95	13	2
1:A:26:THR:O	1:A:44:ILE:HA	0.49	2.08	10	4
1:A:104:CYS:HB2	1:A:113:TRP:CD2	0.49	2.43	12	1
1:A:45:CYS:SG	1:A:50:VAL:O	0.49	2.71	11	2
1:A:107:SER:HB3	1:A:112:ILE:HD12	0.48	1.84	16	1
1:A:63:CYS:HA	1:A:111:VAL:HG23	0.48	1.84	18	1
1:A:85:GLN:HA	1:A:102:ALA:O	0.48	2.09	3	3
1:A:46:LEU:HD12	1:A:52:THR:CG2	0.48	2.37	14	2
1:A:60:ARG:HG3	1:A:82:PHE:CB	0.48	2.38	14	1
1:A:69:PRO:HD3	1:A:74:VAL:HG23	0.48	1.85	10	4
1:A:60:ARG:HG3	1:A:81:GLN:NE2	0.48	2.24	10	1
1:A:15:GLN:CD	1:A:29:ASN:H	0.48	2.16	14	5
1:A:115:GLN:NE2	1:A:118:PRO:HA	0.48	2.24	12	1
1:A:55:LYS:HE2	1:A:56:ASP:OD2	0.48	2.09	19	1
1:A:98:GLY:HA3	1:A:119:ILE:CD1	0.48	2.39	7	2
1:A:30:TYR:CE1	1:A:43:ILE:HD11	0.48	2.44	12	1
1:A:81:GLN:O	1:A:84:SER:HB2	0.48	2.08	1	4
1:A:30:TYR:O	1:A:40:PRO:HB3	0.48	2.08	15	1
1:A:45:CYS:SG	1:A:51:TRP:CZ2	0.48	3.07	10	1
1:A:99:SER:OG	1:A:115:GLN:HA	0.48	2.09	11	1
1:A:24:ILE:HG23	1:A:45:CYS:O	0.47	2.09	1	1
1:A:38:GLY:HA3	1:A:57:ARG:O	0.47	2.09	1	3
1:A:43:ILE:O	1:A:52:THR:HG23	0.47	2.09	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:PHE:HB3	1:A:33:ARG:NE	0.47	2.23	20	1
1:A:54:ALA:C	1:A:57:ARG:HG2	0.47	2.34	20	1
1:A:41:PHE:H	1:A:57:ARG:NH2	0.47	2.06	6	1
1:A:8:LEU:HD23	1:A:11:ALA:HB2	0.47	1.87	7	1
1:A:117:THR:OG1	1:A:118:PRO:HD2	0.47	2.10	13	1
1:A:4:ALA:CB	1:A:20:PHE:HB3	0.47	2.40	4	5
1:A:33:ARG:CZ	1:A:36:TYR:HB2	0.47	2.39	7	1
1:A:102:ALA:HB2	1:A:115:GLN:HB2	0.47	1.86	17	2
1:A:38:GLY:HA2	1:A:59:ARG:NH1	0.47	2.25	7	1
1:A:95:ARG:HB2	1:A:121:ASP:HB3	0.47	1.86	11	2
1:A:36:TYR:HD2	1:A:59:ARG:C	0.47	2.18	7	1
1:A:69:PRO:HG3	1:A:73:MET:C	0.46	2.35	5	2
1:A:96:LEU:HD23	1:A:100:SER:CA	0.46	2.39	5	3
1:A:15:GLN:O	1:A:19:GLU:HG2	0.46	2.09	12	1
1:A:73:MET:SD	1:A:90:CYS:O	0.46	2.73	9	1
1:A:33:ARG:HB2	1:A:36:TYR:CE1	0.46	2.44	18	1
1:A:36:TYR:HH	1:A:82:PHE:HE2	0.46	1.53	7	1
1:A:95:ARG:HB2	1:A:121:ASP:CB	0.46	2.40	8	4
1:A:66:PRO:HD2	1:A:67:PRO:HD3	0.46	1.88	20	1
1:A:12:ARG:N	1:A:13:PRO:HD3	0.46	2.26	7	1
1:A:63:CYS:SG	1:A:81:GLN:C	0.46	2.99	10	1
1:A:90:CYS:CB	1:A:94:TYR:CE2	0.46	2.98	13	1
1:A:34:PRO:C	1:A:106:ILE:HG21	0.46	2.35	14	1
1:A:99:SER:OG	1:A:115:GLN:HG3	0.46	2.11	20	1
1:A:15:GLN:NE2	1:A:29:ASN:N	0.46	2.64	12	5
1:A:81:GLN:CG	1:A:82:PHE:H	0.46	2.24	1	1
1:A:64:ARG:O	1:A:64:ARG:HG3	0.46	2.11	2	1
1:A:39:ARG:HE	1:A:40:PRO:HD2	0.45	1.70	1	1
1:A:63:CYS:SG	1:A:111:VAL:CG2	0.45	3.04	7	1
1:A:65:ASN:H	1:A:66:PRO:HD3	0.45	1.70	4	2
1:A:2:CYS:SG	1:A:51:TRP:CH2	0.45	3.09	6	1
1:A:82:PHE:HA	1:A:104:CYS:SG	0.45	2.51	11	2
1:A:61:LYS:HG2	1:A:62:SER:N	0.45	2.26	20	1
1:A:76:VAL:CG2	1:A:80:ILE:HG13	0.45	2.41	2	1
1:A:102:ALA:HB2	1:A:115:GLN:HB3	0.45	1.88	2	1
1:A:106:ILE:HG22	1:A:108:GLY:N	0.45	2.27	18	5
1:A:94:TYR:CD1	1:A:94:TYR:C	0.45	2.93	17	4
1:A:3:ASN:O	1:A:4:ALA:HB3	0.45	2.10	4	2
1:A:45:CYS:HA	1:A:51:TRP:HA	0.45	1.88	10	1
1:A:121:ASP:O	1:A:122:ARG:C	0.45	2.60	13	4
1:A:5:PRO:O	1:A:6:GLU:HB3	0.45	2.12	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PRO:HG2	1:A:73:MET:N	0.45	2.27	18	2
1:A:5:PRO:HG3	1:A:51:TRP:CZ2	0.45	2.47	13	1
1:A:69:PRO:HG2	1:A:73:MET:C	0.45	2.36	6	2
1:A:45:CYS:SG	1:A:51:TRP:CZ3	0.45	3.10	8	1
1:A:92:LYS:CG	1:A:93:GLY:N	0.45	2.78	20	1
1:A:6:GLU:HG3	1:A:7:TRP:N	0.45	2.27	6	2
1:A:5:PRO:CA	1:A:51:TRP:NE1	0.45	2.80	13	2
1:A:7:TRP:CZ2	1:A:9:PRO:HA	0.45	2.47	11	2
1:A:69:PRO:HB2	1:A:72:GLY:H	0.45	1.72	19	1
1:A:96:LEU:HD13	1:A:100:SER:HA	0.45	1.88	3	2
1:A:64:ARG:O	1:A:64:ARG:HD2	0.45	2.12	5	1
1:A:45:CYS:HB3	1:A:49:SER:C	0.45	2.37	13	1
1:A:33:ARG:NE	1:A:36:TYR:HD1	0.44	2.10	7	1
1:A:41:PHE:CG	1:A:42:SER:N	0.44	2.84	17	1
1:A:76:VAL:HG21	1:A:80:ILE:N	0.44	2.28	8	2
1:A:61:LYS:HB3	1:A:111:VAL:HG13	0.44	1.90	16	2
1:A:86:ILE:HD12	1:A:113:TRP:CZ3	0.44	2.48	17	2
1:A:22:PHE:CE1	1:A:28:LEU:HD21	0.44	2.47	14	3
1:A:44:ILE:O	1:A:51:TRP:HA	0.44	2.12	14	1
1:A:43:ILE:HG13	1:A:51:TRP:CE3	0.44	2.48	14	1
1:A:10:PHE:CD2	1:A:58:CYS:HB2	0.44	2.47	16	2
1:A:32:CYS:SG	1:A:40:PRO:CD	0.44	3.03	2	1
1:A:64:ARG:O	1:A:113:TRP:NE1	0.44	2.50	2	3
1:A:35:GLY:HA3	1:A:106:ILE:CG2	0.44	2.42	13	2
1:A:85:GLN:HG2	1:A:101:SER:OG	0.44	2.12	5	1
1:A:78:LYS:HB2	1:A:84:SER:HB2	0.44	1.89	6	1
1:A:63:CYS:SG	1:A:111:VAL:HG21	0.44	2.52	7	1
1:A:36:TYR:HD1	1:A:59:ARG:C	0.44	2.20	15	1
1:A:77:ILE:HD11	1:A:87:LYS:CD	0.44	2.43	1	1
1:A:22:PHE:CD2	1:A:28:LEU:HD21	0.44	2.47	15	1
1:A:33:ARG:HB2	1:A:34:PRO:CD	0.43	2.43	13	1
1:A:13:PRO:HB3	1:A:30:TYR:CE1	0.43	2.48	20	1
1:A:33:ARG:CZ	1:A:36:TYR:HD1	0.43	2.27	7	1
1:A:98:GLY:CA	1:A:119:ILE:HD13	0.43	2.41	15	1
1:A:15:GLN:HG2	1:A:29:ASN:H	0.43	1.73	20	1
1:A:60:ARG:NH2	1:A:81:GLN:HB3	0.43	2.28	18	1
1:A:95:ARG:N	1:A:95:ARG:HD3	0.43	2.28	3	1
1:A:60:ARG:CD	1:A:81:GLN:HE21	0.43	2.27	8	1
1:A:12:ARG:N	1:A:12:ARG:HD3	0.43	2.29	14	1
1:A:8:LEU:HD21	1:A:10:PHE:CE2	0.43	2.48	18	1
1:A:10:PHE:HB3	1:A:58:CYS:SG	0.43	2.53	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLN:OE1	1:A:28:LEU:HA	0.43	2.13	2	1
1:A:66:PRO:CD	1:A:67:PRO:HD2	0.43	2.43	14	2
1:A:13:PRO:HG3	1:A:30:TYR:CD2	0.43	2.49	10	1
1:A:5:PRO:HG2	1:A:16:LEU:HD12	0.43	1.89	13	1
1:A:79:GLY:O	1:A:80:ILE:HB	0.43	2.13	15	1
1:A:61:LYS:O	1:A:111:VAL:HG11	0.43	2.14	19	1
1:A:60:ARG:HH11	1:A:81:GLN:NE2	0.43	2.12	1	1
1:A:47:LYS:HA	1:A:47:LYS:HE3	0.43	1.90	2	1
1:A:60:ARG:CD	1:A:82:PHE:HB3	0.43	2.44	12	1
1:A:22:PHE:HB3	1:A:26:THR:HG21	0.42	1.91	19	1
1:A:34:PRO:O	1:A:106:ILE:HG13	0.42	2.14	14	1
1:A:67:PRO:HG2	1:A:88:TYR:OH	0.42	2.14	16	1
1:A:10:PHE:CZ	1:A:56:ASP:HA	0.42	2.49	18	1
1:A:81:GLN:O	1:A:84:SER:HB3	0.42	2.14	8	2
1:A:43:ILE:C	1:A:44:ILE:HG13	0.42	2.40	10	1
1:A:22:PHE:CD2	1:A:28:LEU:HD11	0.42	2.48	18	1
1:A:48:ASN:O	1:A:50:VAL:HG23	0.42	2.14	3	1
1:A:44:ILE:HB	1:A:46:LEU:HG	0.42	1.90	18	4
1:A:118:PRO:C	1:A:119:ILE:HG13	0.42	2.38	5	2
1:A:39:ARG:CG	1:A:40:PRO:CD	0.42	2.98	9	1
1:A:115:GLN:HE21	1:A:117:THR:HA	0.42	1.74	13	1
1:A:63:CYS:HA	1:A:111:VAL:CG2	0.42	2.44	18	1
1:A:55:LYS:HE3	1:A:56:ASP:OD1	0.42	2.15	6	1
1:A:14:THR:OG1	1:A:15:GLN:HG3	0.42	2.15	1	1
1:A:87:LYS:HD3	1:A:101:SER:CB	0.42	2.44	8	1
1:A:71:ASN:ND2	1:A:73:MET:HE3	0.42	2.30	9	1
1:A:60:ARG:HG3	1:A:81:GLN:HE21	0.42	1.75	11	1
1:A:13:PRO:HG3	1:A:30:TYR:CE2	0.42	2.50	10	1
1:A:65:ASN:H	1:A:66:PRO:CD	0.42	2.27	13	1
1:A:22:PHE:HB3	1:A:23:PRO:HD2	0.42	1.90	9	1
1:A:3:ASN:HA	1:A:21:GLU:CD	0.42	2.39	16	1
1:A:69:PRO:HG2	1:A:74:VAL:HG23	0.42	1.90	17	1
1:A:37:SER:O	1:A:59:ARG:N	0.42	2.52	7	1
1:A:22:PHE:CG	1:A:26:THR:HG21	0.42	2.48	8	1
1:A:50:VAL:O	1:A:51:TRP:HB2	0.42	2.15	10	1
1:A:19:GLU:C	1:A:21:GLU:H	0.42	2.23	15	1
1:A:55:LYS:HG3	1:A:56:ASP:N	0.42	2.29	18	1
1:A:99:SER:HB3	1:A:101:SER:O	0.42	2.15	3	1
1:A:13:PRO:HB3	1:A:30:TYR:CD1	0.42	2.50	13	3
1:A:15:GLN:HB2	1:A:28:LEU:CD2	0.41	2.45	13	1
1:A:64:ARG:HD2	1:A:64:ARG:C	0.41	2.40	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:MET:SD	1:A:90:CYS:CA	0.41	3.09	14	1
1:A:10:PHE:CD1	1:A:10:PHE:N	0.41	2.87	19	1
1:A:5:PRO:O	1:A:6:GLU:HB2	0.41	2.14	18	2
1:A:33:ARG:CZ	1:A:33:ARG:N	0.41	2.83	7	1
1:A:91:THR:O	1:A:94:TYR:CE1	0.41	2.73	10	1
1:A:76:VAL:CG2	1:A:79:GLY:HA2	0.41	2.45	1	1
1:A:23:PRO:O	1:A:24:ILE:CB	0.41	2.65	19	1
1:A:19:GLU:HB3	1:A:22:PHE:CE2	0.41	2.51	2	1
1:A:39:ARG:HG3	1:A:40:PRO:HD2	0.41	1.92	5	1
1:A:88:TYR:CE1	1:A:115:GLN:OE1	0.41	2.73	10	1
1:A:96:LEU:HD11	1:A:119:ILE:O	0.41	2.15	15	1
1:A:82:PHE:CG	1:A:106:ILE:HD11	0.41	2.51	19	1
1:A:55:LYS:HE3	1:A:56:ASP:CG	0.41	2.40	6	1
1:A:15:GLN:HE22	1:A:28:LEU:CB	0.41	2.28	17	1
1:A:71:ASN:ND2	1:A:90:CYS:O	0.41	2.54	19	1
1:A:35:GLY:C	1:A:106:ILE:HG13	0.41	2.39	4	1
1:A:44:ILE:O	1:A:46:LEU:N	0.41	2.47	6	1
1:A:35:GLY:CA	1:A:108:GLY:HA2	0.41	2.45	12	1
1:A:73:MET:O	1:A:74:VAL:C	0.41	2.63	16	1
1:A:75:HIS:HB2	1:A:87:LYS:HB2	0.41	1.90	16	1
1:A:63:CYS:SG	1:A:113:TRP:CZ2	0.41	3.14	17	1
1:A:60:ARG:HD2	1:A:81:GLN:HE21	0.41	1.76	20	1
1:A:32:CYS:HB3	1:A:36:TYR:HB2	0.41	1.93	2	1
1:A:95:ARG:HD2	1:A:121:ASP:OD2	0.41	2.15	6	1
1:A:26:THR:O	1:A:44:ILE:HG23	0.41	2.15	10	1
1:A:99:SER:HB3	1:A:115:GLN:HG3	0.41	1.93	16	1
1:A:85:GLN:HE21	1:A:101:SER:CB	0.41	2.29	5	1
1:A:16:LEU:HD23	1:A:16:LEU:C	0.41	2.41	8	1
1:A:74:VAL:HG23	1:A:87:LYS:O	0.41	2.16	14	1
1:A:40:PRO:HA	1:A:57:ARG:HH21	0.41	1.76	15	1
1:A:13:PRO:CG	1:A:30:TYR:CE1	0.41	3.04	17	1
1:A:33:ARG:HH22	1:A:36:TYR:HB2	0.40	1.71	7	1
1:A:94:TYR:CG	1:A:95:ARG:N	0.40	2.87	13	1
1:A:44:ILE:CD1	1:A:52:THR:HG21	0.40	2.44	15	1
1:A:5:PRO:HG3	1:A:43:ILE:CD1	0.40	2.46	17	1
1:A:12:ARG:CG	1:A:33:ARG:HB3	0.40	2.46	7	1
1:A:95:ARG:O	1:A:121:ASP:CB	0.40	2.69	7	1
1:A:22:PHE:HD2	1:A:26:THR:HG21	0.40	1.75	14	1
1:A:97:ILE:HB	1:A:119:ILE:CG2	0.40	2.47	15	1
1:A:76:VAL:HG12	1:A:79:GLY:H	0.40	1.76	11	1
1:A:99:SER:HB2	1:A:115:GLN:HG3	0.40	1.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:CYS:SG	1:A:111:VAL:HB	0.40	2.57	18	1
1:A:36:TYR:O	1:A:39:ARG:NH1	0.40	2.54	14	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	120/128 (94%)	104±2 (87±2%)	9±2 (7±2%)	7±1 (6±1%)	2	20
All	All	2400/2560 (94%)	2089 (87%)	173 (7%)	138 (6%)	2	20

All 21 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	4	ALA	20
1	A	68	ASP	19
1	A	80	ILE	19
1	A	6	GLU	17
1	A	117	THR	13
1	A	45	CYS	11
1	A	50	VAL	7
1	A	53	GLY	6
1	A	65	ASN	5
1	A	5	PRO	5
1	A	51	TRP	3
1	A	33	ARG	2
1	A	24	ILE	2
1	A	56	ASP	2
1	A	54	ALA	1
1	A	76	VAL	1
1	A	39	ARG	1
1	A	44	ILE	1
1	A	74	VAL	1
1	A	41	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LYS	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	108/110 (98%)	101±1 (93±1%)	7±1 (7±1%)	17	66
All	All	2160/2200 (98%)	2019 (93%)	141 (7%)	17	66

All 34 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	105	ILE	20
1	A	15	GLN	11
1	A	65	ASN	8
1	A	12	ARG	7
1	A	16	LEU	7
1	A	45	CYS	7
1	A	33	ARG	6
1	A	86	ILE	6
1	A	39	ARG	5
1	A	112	ILE	5
1	A	1	GLN	5
1	A	63	CYS	5
1	A	10	PHE	4
1	A	68	ASP	4
1	A	104	CYS	4
1	A	117	THR	4
1	A	44	ILE	4
1	A	47	LYS	3
1	A	49	SER	3
1	A	87	LYS	3
1	A	2	CYS	2
1	A	52	THR	2
1	A	94	TYR	2
1	A	60	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	64	ARG	2
1	A	3	ASN	2
1	A	28	LEU	1
1	A	95	ARG	1
1	A	24	ILE	1
1	A	14	THR	1
1	A	99	SER	1
1	A	43	ILE	1
1	A	66	PRO	1
1	A	115	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% 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	1370
Number of shifts mapped to atoms	1365
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 5 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	GLY	H	8.3724	.	1
1	A	0	GLY	HA2	3.9244	.	.
1	A	0	GLY	C	176.2039	.	1
1	A	0	GLY	CA	45.3931	.	1
1	A	0	GLY	N	108.0758	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	121	0.21 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	-0.03 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	117	0.90 ± 0.24	Should be applied

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
^{15}N	113	0.33 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1365 atoms were assigned a chemical shift out of a possible 1640. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	590/600 (98%)	242/244 (99%)	236/244 (97%)	112/112 (100%)
Sidechain	659/902 (73%)	429/583 (74%)	225/276 (82%)	5/43 (12%)
Aromatic	116/138 (84%)	58/67 (87%)	55/67 (82%)	3/4 (75%)
Overall	1365/1640 (83%)	729/894 (82%)	516/587 (88%)	120/159 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1365 atoms were assigned a chemical shift out of a possible 1640. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	590/600 (98%)	242/244 (99%)	236/244 (97%)	112/112 (100%)
Sidechain	659/902 (73%)	429/583 (74%)	225/276 (82%)	5/43 (12%)
Aromatic	116/138 (84%)	58/67 (87%)	55/67 (82%)	3/4 (75%)
Overall	1365/1640 (83%)	729/894 (82%)	516/587 (88%)	120/159 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

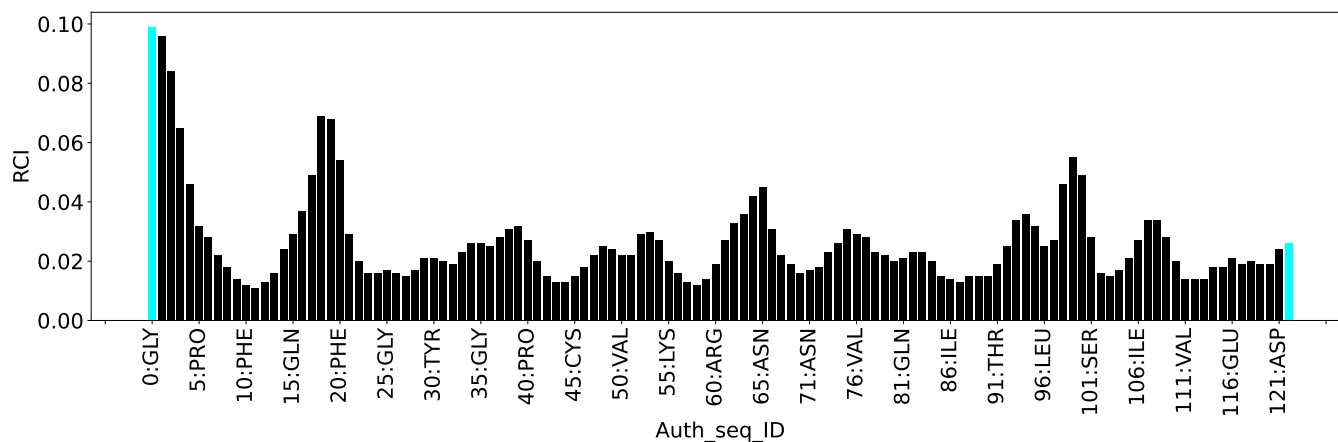
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	57	ARG	HG2	0.05	0.26 – 2.87	-5.8
1	A	5	PRO	HG2	0.21	0.41 – 3.45	-5.7
1	A	8	LEU	HB3	-0.27	-0.26 – 3.31	-5.0

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

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

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2578
Intra-residue ($ i-j =0$)	507
Sequential ($ i-j =1$)	724
Medium range ($ i-j >1$ and $ i-j <5$)	348
Long range ($ i-j \geq 5$)	999
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	13
Number of restraints per residue	20.1
Number of long range restraints per residue ¹	7.8

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)	74.4	0.2
0.2-0.5 (Medium)	78.7	0.5
>0.5 (Large)	14.3	1.06

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 ⓘ

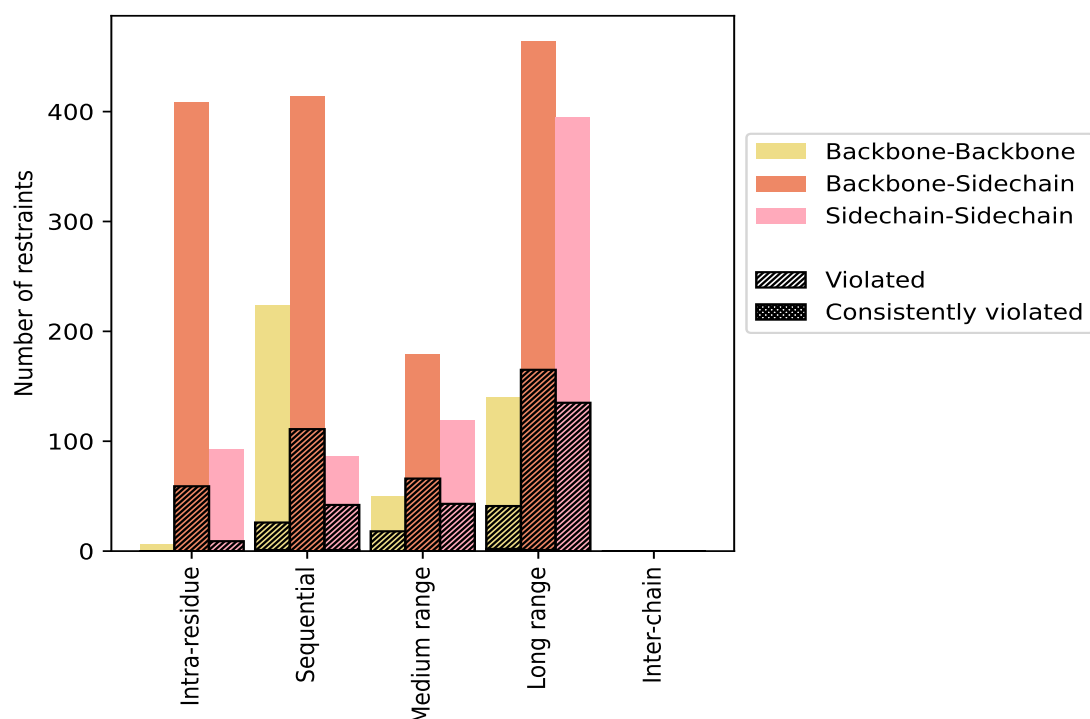
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	507	19.7	68	13.4	2.6	0	0.0	0.0
Backbone-Backbone	6	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	408	15.8	59	14.5	2.3	0	0.0	0.0
Sidechain-Sidechain	93	3.6	9	9.7	0.3	0	0.0	0.0
Sequential ($i-j =1$)	724	28.1	179	24.7	6.9	2	0.3	0.1
Backbone-Backbone	224	8.7	26	11.6	1.0	1	0.4	0.0
Backbone-Sidechain	414	16.1	111	26.8	4.3	0	0.0	0.0
Sidechain-Sidechain	86	3.3	42	48.8	1.6	1	1.2	0.0
Medium range ($i-j >1$ & $i-j <5$)	348	13.5	127	36.5	4.9	0	0.0	0.0
Backbone-Backbone	50	1.9	18	36.0	0.7	0	0.0	0.0
Backbone-Sidechain	179	6.9	66	36.9	2.6	0	0.0	0.0
Sidechain-Sidechain	119	4.6	43	36.1	1.7	0	0.0	0.0
Long range ($i-j \geq 5$)	999	38.8	341	34.1	13.2	3	0.3	0.1
Backbone-Backbone	140	5.4	41	29.3	1.6	2	1.4	0.1
Backbone-Sidechain	464	18.0	165	35.6	6.4	1	0.2	0.0
Sidechain-Sidechain	395	15.3	135	34.2	5.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2578	100.0	715	27.7	27.7	5	0.2	0.2
Backbone-Backbone	420	16.3	85	20.2	3.3	3	0.7	0.1
Backbone-Sidechain	1465	56.8	401	27.4	15.6	1	0.1	0.0
Sidechain-Sidechain	693	26.9	229	33.0	8.9	1	0.1	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	14	54	33	87	0	188	0.27	0.87	0.15	0.22
2	12	49	30	90	0	181	0.24	0.92	0.13	0.21
3	15	47	30	80	0	172	0.26	0.99	0.15	0.21
4	17	42	35	86	0	180	0.26	1.06	0.15	0.22
5	19	46	30	66	0	161	0.25	0.89	0.13	0.23
6	10	43	30	79	0	162	0.26	0.87	0.16	0.2
7	17	46	36	79	0	178	0.27	0.95	0.15	0.23
8	17	47	28	89	0	181	0.26	0.94	0.16	0.22
9	16	37	32	63	0	148	0.27	1.05	0.16	0.22
10	14	38	29	83	0	164	0.26	0.77	0.15	0.22

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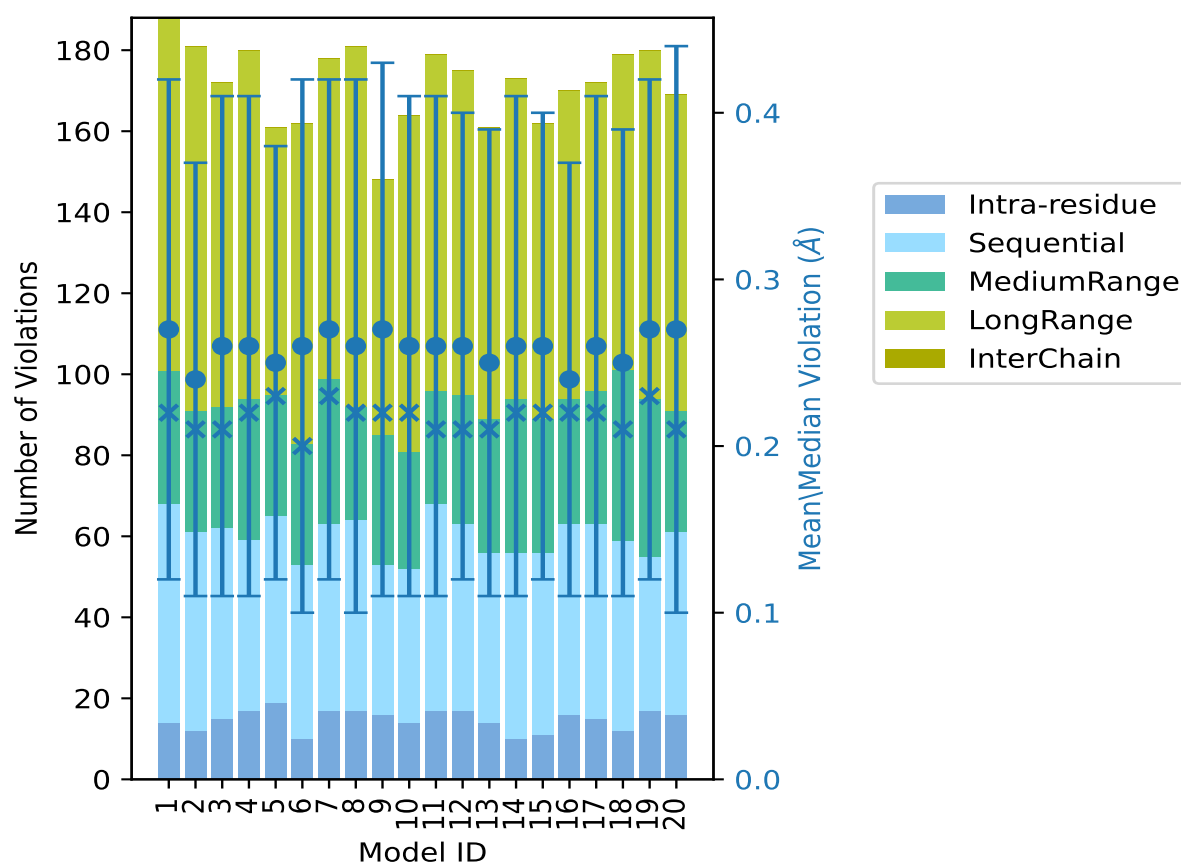
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	17	51	28	83	0	179	0.26	0.79	0.15	0.21
12	17	46	32	80	0	175	0.26	0.72	0.14	0.21
13	14	42	33	72	0	161	0.25	0.83	0.14	0.21
14	10	46	38	79	0	173	0.26	1.05	0.15	0.22
15	11	45	33	73	0	162	0.26	0.68	0.14	0.22
16	16	47	31	76	0	170	0.24	0.72	0.13	0.22
17	15	48	33	76	0	172	0.26	0.84	0.15	0.22
18	12	47	42	78	0	179	0.25	0.87	0.14	0.21
19	17	38	39	86	0	180	0.27	0.8	0.15	0.23
20	16	45	30	78	0	169	0.27	0.95	0.17	0.21

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

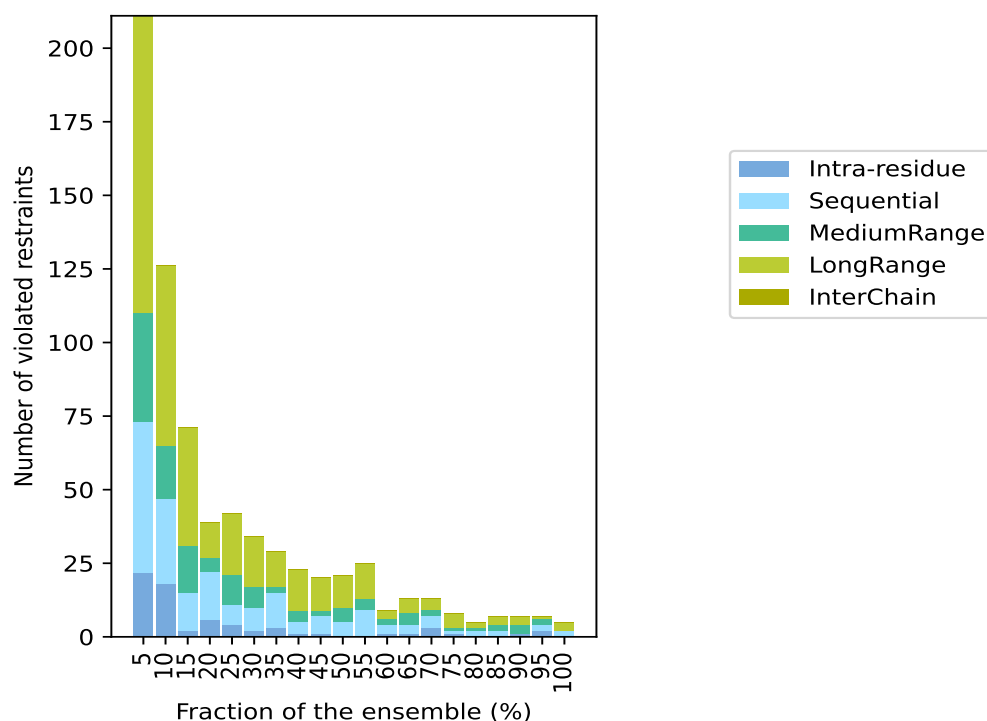
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1863(IR:439, SQ:545, MR:221, LR:658, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
22	51	37	101	0	211	1	5.0
18	29	18	61	0	126	2	10.0
2	13	16	40	0	71	3	15.0
6	16	5	12	0	39	4	20.0
4	7	10	21	0	42	5	25.0
2	8	7	17	0	34	6	30.0
3	12	2	12	0	29	7	35.0
1	4	4	14	0	23	8	40.0
1	6	2	11	0	20	9	45.0
0	5	5	11	0	21	10	50.0
0	9	4	12	0	25	11	55.0
1	3	2	3	0	9	12	60.0
1	3	4	5	0	13	13	65.0
3	4	2	4	0	13	14	70.0
1	1	1	5	0	8	15	75.0
0	2	1	2	0	5	16	80.0
0	2	2	3	0	7	17	85.0
1	0	3	3	0	7	18	90.0
2	2	2	1	0	7	19	95.0
0	2	0	3	0	5	20	100.0

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

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

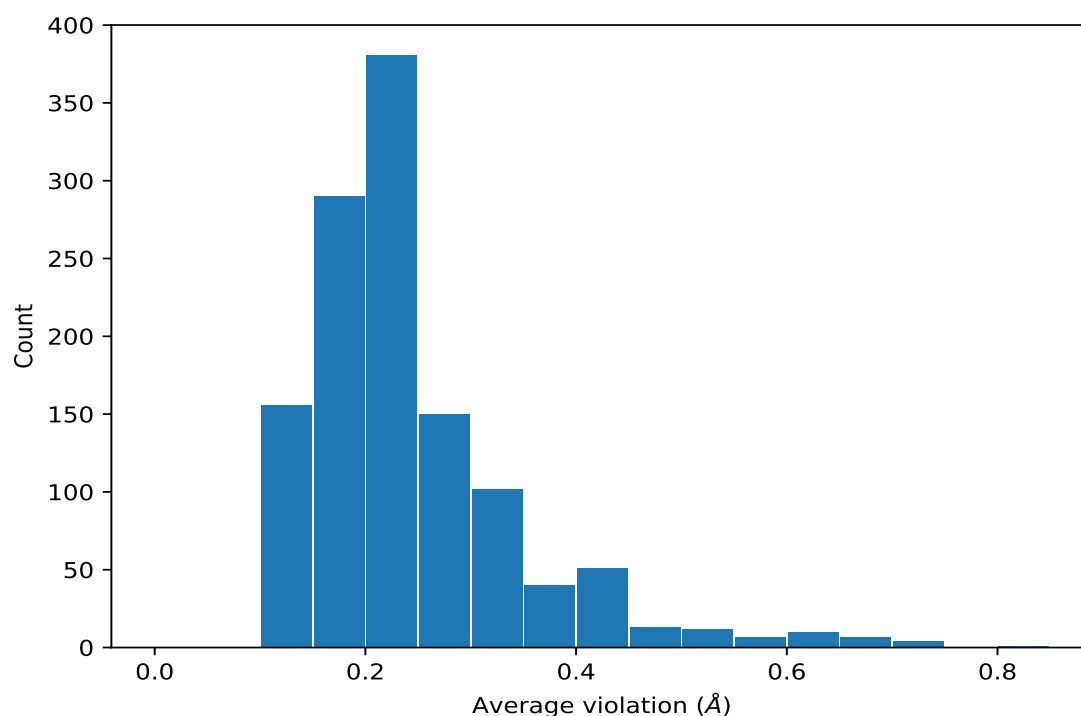
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	20	0.52	0.12	0.5
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	20	0.4	0.18	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	20	0.4	0.18	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	20	0.4	0.18	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	20	0.4	0.18	0.32
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	20	0.37	0.1	0.36
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	20	0.3	0.1	0.28
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	20	0.26	0.05	0.26
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	19	0.57	0.2	0.57
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	19	0.4	0.13	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	19	0.4	0.13	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	19	0.4	0.13	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	19	0.4	0.13	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	19	0.4	0.13	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	19	0.4	0.13	0.38
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	19	0.35	0.1	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	19	0.34	0.14	0.29
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	19	0.32	0.04	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	19	0.32	0.04	0.32
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	19	0.3	0.06	0.31
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	19	0.23	0.07	0.23
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	19	0.23	0.07	0.23
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	19	0.23	0.07	0.23
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	18	0.42	0.17	0.43
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	18	0.42	0.17	0.43
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	18	0.4	0.11	0.42
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	18	0.4	0.11	0.42
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	18	0.28	0.12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	18	0.26	0.06	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	18	0.26	0.06	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	18	0.26	0.06	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	18	0.26	0.06	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	18	0.26	0.06	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	18	0.26	0.06	0.26
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	18	0.25	0.09	0.24
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	18	0.25	0.09	0.24
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	18	0.22	0.08	0.2
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	18	0.21	0.07	0.2
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	18	0.21	0.07	0.2
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	18	0.21	0.07	0.2
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	17	0.39	0.11	0.38
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	17	0.32	0.09	0.34
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	17	0.28	0.09	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	17	0.28	0.09	0.27
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	17	0.25	0.11	0.21
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	17	0.25	0.11	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	17	0.23	0.11	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	17	0.23	0.11	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	17	0.2	0.07	0.2
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	17	0.2	0.07	0.2
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	17	0.17	0.04	0.17
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	16	0.28	0.1	0.31
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	16	0.28	0.1	0.31
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	16	0.25	0.1	0.22
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	16	0.23	0.08	0.22
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	16	0.23	0.08	0.22
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	16	0.23	0.08	0.22
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	16	0.23	0.1	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	16	0.23	0.1	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	16	0.23	0.1	0.2
(1,952)	1:107:A:SER:H	1:110:A:THR:H	16	0.22	0.08	0.22
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	15	0.46	0.15	0.48
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	15	0.46	0.15	0.48
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	15	0.39	0.16	0.44
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	15	0.35	0.16	0.39
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	15	0.35	0.16	0.39
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	15	0.35	0.16	0.39
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	15	0.35	0.16	0.39
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	15	0.3	0.1	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	15	0.3	0.1	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	15	0.3	0.1	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	15	0.3	0.1	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	15	0.3	0.1	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	15	0.3	0.1	0.29
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	15	0.29	0.13	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	15	0.28	0.12	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	15	0.28	0.12	0.27
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	15	0.28	0.13	0.26
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	15	0.22	0.07	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	15	0.22	0.07	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	15	0.22	0.07	0.22
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	14	0.62	0.05	0.61
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	14	0.57	0.05	0.58
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	14	0.57	0.05	0.58
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	14	0.51	0.1	0.51
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	14	0.51	0.1	0.51
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	14	0.51	0.1	0.51
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	14	0.51	0.1	0.51
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	14	0.51	0.1	0.51
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	14	0.51	0.1	0.51
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	14	0.44	0.16	0.5
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	14	0.44	0.16	0.5
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	14	0.44	0.16	0.5
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	14	0.39	0.08	0.42
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	14	0.39	0.08	0.42
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	14	0.32	0.11	0.31
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	14	0.29	0.13	0.24
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	14	0.29	0.13	0.24
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	14	0.24	0.06	0.22
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	14	0.24	0.06	0.22
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	14	0.24	0.06	0.22
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	14	0.24	0.13	0.18
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	14	0.24	0.13	0.18
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	14	0.24	0.07	0.25
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	14	0.24	0.05	0.22
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	14	0.19	0.06	0.16
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	14	0.19	0.05	0.2
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	13	0.62	0.16	0.66
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	13	0.62	0.16	0.66
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	13	0.57	0.31	0.77
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	13	0.57	0.31	0.77
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	13	0.49	0.09	0.51
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	13	0.38	0.11	0.4
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	13	0.35	0.13	0.35
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	13	0.32	0.16	0.28
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	13	0.32	0.16	0.28
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	13	0.32	0.11	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	13	0.26	0.14	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	13	0.26	0.14	0.22
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	13	0.23	0.08	0.21
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	13	0.22	0.06	0.18
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	13	0.21	0.07	0.21
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	13	0.21	0.07	0.21
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	13	0.19	0.05	0.19
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	13	0.16	0.04	0.16
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	12	0.34	0.07	0.35
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	12	0.29	0.06	0.29
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	12	0.29	0.06	0.29
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	12	0.24	0.1	0.19
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	12	0.23	0.08	0.22
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	12	0.23	0.08	0.22
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	12	0.21	0.06	0.2
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	12	0.21	0.06	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	12	0.21	0.07	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	12	0.21	0.07	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	12	0.21	0.07	0.2
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	12	0.2	0.08	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	12	0.2	0.08	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	12	0.2	0.08	0.19
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	12	0.16	0.04	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	12	0.16	0.04	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	12	0.16	0.04	0.16
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	12	0.14	0.04	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	12	0.14	0.04	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	12	0.14	0.04	0.12
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	11	0.4	0.24	0.3
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	11	0.4	0.24	0.3
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	11	0.4	0.19	0.3
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	11	0.36	0.17	0.36
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	11	0.36	0.17	0.36
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	11	0.33	0.24	0.24
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	11	0.32	0.1	0.31
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	11	0.32	0.1	0.31
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	11	0.32	0.1	0.31
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	11	0.28	0.13	0.24
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	11	0.27	0.14	0.21
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	11	0.27	0.06	0.28
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	11	0.27	0.06	0.28
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	11	0.27	0.06	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	11	0.25	0.05	0.27
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	11	0.24	0.07	0.23
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	11	0.24	0.07	0.23
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	11	0.24	0.07	0.21
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	11	0.24	0.07	0.21
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	11	0.24	0.07	0.24
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	11	0.24	0.07	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	11	0.24	0.07	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	11	0.24	0.07	0.24
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	11	0.23	0.09	0.22
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	11	0.23	0.09	0.22
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	11	0.23	0.07	0.22
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	11	0.23	0.07	0.21
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	11	0.23	0.07	0.21
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	11	0.23	0.1	0.21
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	11	0.23	0.1	0.21
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	11	0.23	0.1	0.21
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	11	0.23	0.1	0.21
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	11	0.22	0.09	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	11	0.22	0.09	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	11	0.22	0.09	0.19
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	11	0.22	0.07	0.2
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	11	0.22	0.09	0.18
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	11	0.22	0.09	0.18
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	11	0.22	0.09	0.18
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	11	0.21	0.09	0.19
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	11	0.21	0.09	0.19
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	11	0.21	0.09	0.19
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	11	0.21	0.09	0.19
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	11	0.21	0.13	0.17
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	11	0.21	0.13	0.17
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	11	0.19	0.07	0.2
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	11	0.19	0.08	0.17
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	11	0.18	0.07	0.16
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	11	0.15	0.04	0.15
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	10	0.64	0.13	0.61
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	10	0.46	0.28	0.43
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	10	0.3	0.13	0.3
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	10	0.28	0.08	0.29
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	10	0.28	0.08	0.29
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	10	0.28	0.08	0.29
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	10	0.28	0.14	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	10	0.27	0.13	0.25
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	10	0.27	0.13	0.25
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	10	0.27	0.13	0.25
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	10	0.25	0.06	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	10	0.25	0.06	0.26
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	10	0.25	0.08	0.26
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	10	0.25	0.08	0.26
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	10	0.25	0.08	0.26
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	10	0.24	0.12	0.2
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	10	0.23	0.07	0.24
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	10	0.22	0.07	0.22
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	10	0.22	0.07	0.22
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	10	0.2	0.08	0.18
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	10	0.2	0.07	0.17
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	10	0.2	0.07	0.17
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	10	0.2	0.07	0.17
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	10	0.2	0.07	0.17
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	10	0.2	0.07	0.17
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	10	0.2	0.07	0.17
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	10	0.19	0.08	0.18
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	10	0.19	0.08	0.18
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	10	0.19	0.05	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	10	0.19	0.05	0.2
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	10	0.18	0.07	0.15
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	10	0.18	0.06	0.16
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	10	0.18	0.06	0.16
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	10	0.18	0.07	0.15
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	10	0.16	0.03	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	10	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	10	0.15	0.03	0.15
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	10	0.15	0.03	0.15
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	9	0.67	0.03	0.67
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	9	0.67	0.03	0.67
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	9	0.36	0.24	0.27
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	9	0.36	0.24	0.27
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	9	0.32	0.08	0.34
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	9	0.32	0.08	0.34
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	9	0.3	0.06	0.31
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	9	0.3	0.06	0.31
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	9	0.3	0.06	0.31
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	9	0.29	0.14	0.27
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	9	0.29	0.14	0.27
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	9	0.28	0.13	0.33
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	9	0.26	0.11	0.23
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	9	0.26	0.11	0.23
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	9	0.26	0.11	0.23
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	9	0.26	0.09	0.26
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	9	0.26	0.08	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	9	0.26	0.08	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	9	0.26	0.08	0.21
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	9	0.25	0.03	0.27
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	9	0.25	0.03	0.27
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	9	0.23	0.07	0.21
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	9	0.22	0.06	0.2
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	9	0.2	0.07	0.17
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	9	0.18	0.05	0.16
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	9	0.17	0.05	0.15
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	9	0.17	0.04	0.17
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	9	0.17	0.06	0.15
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	9	0.17	0.04	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	9	0.17	0.04	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	9	0.17	0.04	0.19
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	9	0.15	0.05	0.14
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	9	0.14	0.04	0.13
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	8	0.4	0.25	0.42
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	8	0.4	0.25	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	8	0.38	0.1	0.41
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	8	0.38	0.15	0.34
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	8	0.36	0.22	0.3
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	8	0.36	0.22	0.3
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	8	0.36	0.22	0.3
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	8	0.33	0.13	0.29
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	8	0.33	0.13	0.29
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	8	0.32	0.14	0.3
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	8	0.24	0.09	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	8	0.23	0.08	0.22
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	8	0.23	0.08	0.22
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	8	0.23	0.08	0.22
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	8	0.21	0.07	0.2
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	8	0.21	0.11	0.17
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	8	0.21	0.11	0.17
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	8	0.21	0.1	0.18
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	8	0.21	0.1	0.18
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	8	0.21	0.1	0.18
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	8	0.21	0.1	0.18
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	8	0.21	0.1	0.18
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	8	0.21	0.1	0.18
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	8	0.2	0.07	0.18
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	8	0.2	0.07	0.18
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	8	0.2	0.07	0.18
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	8	0.2	0.09	0.15
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	8	0.19	0.09	0.16
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	8	0.19	0.09	0.16
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	8	0.19	0.09	0.16
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	8	0.18	0.08	0.15
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	8	0.18	0.05	0.16
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	8	0.18	0.06	0.16
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	8	0.17	0.05	0.17
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	8	0.17	0.05	0.17
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	8	0.17	0.05	0.17
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	8	0.17	0.02	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	8	0.17	0.02	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	8	0.17	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	8	0.16	0.05	0.16
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	8	0.16	0.05	0.16
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	8	0.16	0.05	0.16
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	8	0.16	0.03	0.16
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	8	0.16	0.03	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	8	0.16	0.05	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	8	0.16	0.05	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	8	0.16	0.05	0.16
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	8	0.16	0.07	0.14
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	7	0.73	0.27	0.87
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	7	0.73	0.27	0.87
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	7	0.73	0.27	0.87
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	7	0.43	0.18	0.49
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	7	0.38	0.21	0.32
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	7	0.38	0.21	0.32
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	7	0.37	0.13	0.35
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	7	0.37	0.13	0.35
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	7	0.37	0.13	0.35
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	7	0.35	0.12	0.38
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	7	0.3	0.05	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	7	0.3	0.05	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	7	0.3	0.05	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	7	0.3	0.05	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	7	0.3	0.05	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	7	0.3	0.05	0.29
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	7	0.28	0.07	0.3
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	7	0.26	0.12	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	7	0.26	0.11	0.21
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	7	0.26	0.11	0.21
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	7	0.26	0.11	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	7	0.26	0.15	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	7	0.26	0.15	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	7	0.26	0.15	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	7	0.26	0.15	0.21
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	7	0.24	0.06	0.23
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	7	0.24	0.06	0.23
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	7	0.23	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	7	0.23	0.06	0.24
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	7	0.22	0.09	0.2
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	7	0.22	0.09	0.2
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	7	0.21	0.07	0.25
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	7	0.21	0.07	0.25
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	7	0.21	0.07	0.25
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	7	0.21	0.07	0.25
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	7	0.21	0.07	0.25
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	7	0.21	0.07	0.22
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	7	0.21	0.08	0.22
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	7	0.21	0.05	0.21
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	7	0.2	0.05	0.2
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	7	0.2	0.07	0.17
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	7	0.18	0.04	0.21
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	7	0.18	0.07	0.18
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	7	0.18	0.07	0.18
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	7	0.18	0.07	0.18
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	7	0.18	0.05	0.19
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	7	0.18	0.04	0.17
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	7	0.18	0.04	0.17
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	7	0.18	0.04	0.17
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	7	0.17	0.06	0.16
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	7	0.16	0.04	0.18
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	7	0.16	0.05	0.14
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	7	0.16	0.05	0.14
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	7	0.14	0.03	0.15
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	7	0.14	0.04	0.13
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	7	0.14	0.04	0.13
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	7	0.14	0.04	0.13
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	6	0.42	0.15	0.45
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	6	0.42	0.15	0.45
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	6	0.3	0.15	0.24
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	6	0.3	0.15	0.24
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	6	0.27	0.14	0.25
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	6	0.25	0.14	0.2
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	6	0.24	0.06	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	6	0.24	0.06	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	6	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	6	0.24	0.06	0.24
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	6	0.24	0.06	0.24
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	6	0.24	0.07	0.23
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	6	0.24	0.07	0.23
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	6	0.24	0.07	0.23
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	6	0.23	0.13	0.18
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	6	0.23	0.13	0.18
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	6	0.23	0.13	0.18
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	6	0.23	0.13	0.18
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	6	0.23	0.13	0.18
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	6	0.23	0.13	0.18
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	6	0.22	0.08	0.2
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	6	0.22	0.08	0.2
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	6	0.22	0.06	0.22
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	6	0.22	0.06	0.22
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	6	0.21	0.1	0.18
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	6	0.21	0.1	0.18
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	6	0.21	0.1	0.17
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	6	0.21	0.07	0.2
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	6	0.21	0.08	0.21
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	6	0.2	0.05	0.2
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	6	0.2	0.05	0.2
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	6	0.2	0.05	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	6	0.2	0.05	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	6	0.2	0.05	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	6	0.2	0.05	0.2
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	6	0.2	0.04	0.22
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	6	0.2	0.04	0.22
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	6	0.19	0.1	0.16
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	6	0.19	0.1	0.16
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	6	0.19	0.1	0.16
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	6	0.19	0.07	0.2
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	6	0.19	0.05	0.18
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	6	0.19	0.06	0.17
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	6	0.19	0.06	0.17
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	6	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	6	0.19	0.06	0.17
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	6	0.19	0.06	0.17
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	6	0.19	0.06	0.17
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	6	0.19	0.05	0.18
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	6	0.19	0.05	0.18
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	6	0.19	0.03	0.18
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	6	0.19	0.03	0.18
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	6	0.19	0.06	0.18
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	6	0.19	0.06	0.18
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	6	0.19	0.06	0.18
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	6	0.19	0.08	0.16
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	6	0.18	0.07	0.16
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	6	0.18	0.07	0.16
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	6	0.18	0.07	0.16
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	6	0.17	0.07	0.14
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	6	0.17	0.07	0.14
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	6	0.17	0.07	0.14
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	6	0.17	0.07	0.14
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	6	0.16	0.05	0.14
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	6	0.16	0.05	0.14
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	6	0.16	0.05	0.14
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	6	0.16	0.05	0.14
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	6	0.16	0.05	0.14
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	6	0.16	0.05	0.14
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	6	0.16	0.04	0.16
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	6	0.16	0.07	0.14
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	6	0.16	0.07	0.14
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	6	0.15	0.04	0.15
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	6	0.15	0.04	0.14
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	6	0.14	0.02	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	6	0.14	0.02	0.15
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	6	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	6	0.13	0.03	0.13
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	6	0.12	0.02	0.12
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	6	0.12	0.02	0.12
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	6	0.12	0.02	0.12
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	5	0.72	0.09	0.76
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	5	0.64	0.06	0.63
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	5	0.64	0.06	0.63
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	5	0.53	0.22	0.62
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	5	0.45	0.13	0.44
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	5	0.45	0.13	0.44
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	5	0.41	0.12	0.37
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	5	0.41	0.12	0.37
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	5	0.39	0.16	0.33
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	5	0.32	0.13	0.31
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	5	0.32	0.13	0.31
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	5	0.31	0.2	0.25
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	5	0.31	0.2	0.25
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	5	0.31	0.14	0.25
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	5	0.31	0.14	0.25
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	5	0.31	0.14	0.25
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	5	0.31	0.14	0.25
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	5	0.29	0.12	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	5	0.29	0.12	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	5	0.29	0.12	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	5	0.29	0.12	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	5	0.29	0.12	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	5	0.29	0.12	0.29
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	5	0.26	0.09	0.25
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	5	0.26	0.09	0.25
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	5	0.26	0.09	0.25
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	5	0.25	0.06	0.25
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	5	0.24	0.08	0.28
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	5	0.24	0.08	0.28
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	5	0.24	0.09	0.21
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	5	0.24	0.11	0.26
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	5	0.24	0.11	0.26
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	5	0.24	0.11	0.26
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	5	0.24	0.11	0.26
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	5	0.23	0.05	0.2
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	5	0.23	0.05	0.2
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	5	0.23	0.05	0.2
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	5	0.23	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	5	0.22	0.09	0.24
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	5	0.22	0.09	0.24
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	5	0.22	0.05	0.23
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	5	0.22	0.05	0.23
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	5	0.22	0.05	0.23
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	5	0.22	0.08	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	5	0.22	0.08	0.2
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	5	0.22	0.07	0.18
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	5	0.22	0.07	0.18
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	5	0.21	0.1	0.16
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	5	0.21	0.1	0.16
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	5	0.2	0.07	0.17
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	5	0.2	0.07	0.17
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	5	0.2	0.06	0.18
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	5	0.2	0.06	0.18
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	5	0.2	0.04	0.2
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	5	0.2	0.07	0.16
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	5	0.2	0.07	0.16
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	5	0.2	0.07	0.16
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	5	0.2	0.07	0.16
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	5	0.19	0.04	0.17
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	5	0.19	0.04	0.17
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	5	0.19	0.06	0.16
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	5	0.19	0.06	0.16
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	5	0.19	0.06	0.15
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	5	0.19	0.05	0.21
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	5	0.18	0.05	0.19
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	5	0.18	0.05	0.19
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	5	0.18	0.1	0.16
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	5	0.18	0.07	0.17
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	5	0.18	0.07	0.17
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	5	0.18	0.06	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	5	0.18	0.06	0.16
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	5	0.17	0.06	0.14
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	5	0.17	0.03	0.17
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	5	0.17	0.06	0.13
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	5	0.17	0.04	0.17
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	5	0.17	0.04	0.17
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	5	0.15	0.03	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	5	0.15	0.03	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	5	0.15	0.03	0.13
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	5	0.15	0.04	0.14
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	5	0.14	0.02	0.14
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	5	0.14	0.04	0.13
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	5	0.14	0.04	0.13
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	5	0.14	0.04	0.13
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	5	0.12	0.02	0.11
(1,533)	1:89:A:SER:HA	1:91:A:THR:H	4	0.65	0.21	0.74
(1,554)	1:87:A:LYS:HG3	1:88:A:TYR:H	4	0.6	0.04	0.6
(1,1499)	1:58:A:CYS:HA	1:59:A:ARG:HD3	4	0.48	0.04	0.48
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG2	4	0.48	0.25	0.52
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG3	4	0.48	0.25	0.52
(1,148)	1:74:A:VAL:HG11	1:89:A:SER:H	4	0.35	0.14	0.32
(1,148)	1:74:A:VAL:HG12	1:89:A:SER:H	4	0.35	0.14	0.32
(1,148)	1:74:A:VAL:HG13	1:89:A:SER:H	4	0.35	0.14	0.32
(1,771)	1:51:A:TRP:H	1:51:A:TRP:HB2	4	0.32	0.05	0.31
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB2	4	0.31	0.09	0.32
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB3	4	0.31	0.09	0.32
(1,2134)	1:41:A:PHE:HB2	1:42:A:SER:H	4	0.29	0.11	0.33
(1,2134)	1:41:A:PHE:HB3	1:42:A:SER:H	4	0.29	0.11	0.33
(1,2165)	1:47:A:LYS:HG2	1:49:A:SER:H	4	0.29	0.09	0.33
(1,2165)	1:47:A:LYS:HG3	1:49:A:SER:H	4	0.29	0.09	0.33
(1,1129)	1:122:A:ARG:H	1:122:A:ARG:HB3	4	0.26	0.05	0.26
(1,790)	1:16:A:LEU:H	1:28:A:LEU:HG	4	0.26	0.11	0.2
(1,2055)	1:16:A:LEU:HD11	1:17:A:THR:HA	4	0.25	0.03	0.26
(1,2055)	1:16:A:LEU:HD12	1:17:A:THR:HA	4	0.25	0.03	0.26
(1,2055)	1:16:A:LEU:HD13	1:17:A:THR:HA	4	0.25	0.03	0.26
(1,2055)	1:16:A:LEU:HD21	1:17:A:THR:HA	4	0.25	0.03	0.26
(1,2055)	1:16:A:LEU:HD22	1:17:A:THR:HA	4	0.25	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2055)	1:16:A:LEU:HD23	1:17:A:THR:HA	4	0.25	0.03	0.26
(1,261)	1:54:A:ALA:H	1:55:A:LYS:H	4	0.24	0.12	0.22
(1,1096)	1:17:A:THR:HG21	1:19:A:GLU:HG3	4	0.24	0.08	0.22
(1,1096)	1:17:A:THR:HG22	1:19:A:GLU:HG3	4	0.24	0.08	0.22
(1,1096)	1:17:A:THR:HG23	1:19:A:GLU:HG3	4	0.24	0.08	0.22
(1,795)	1:18:A:ASP:H	1:19:A:GLU:HG3	4	0.23	0.12	0.19
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB2	4	0.21	0.1	0.16
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB3	4	0.21	0.1	0.16
(1,161)	1:14:A:THR:H	1:29:A:ASN:H	4	0.21	0.1	0.16
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD11	4	0.2	0.02	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD12	4	0.2	0.02	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD13	4	0.2	0.02	0.22
(1,628)	1:77:A:ILE:H	1:86:A:ILE:HB	4	0.2	0.06	0.21
(1,862)	1:13:A:PRO:HA	1:31:A:GLU:H	4	0.2	0.07	0.2
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	4	0.2	0.01	0.2
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	4	0.2	0.01	0.2
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	4	0.2	0.01	0.2
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	4	0.2	0.01	0.2
(1,1629)	1:87:A:LYS:HA	1:87:A:LYS:HG3	4	0.2	0.02	0.2
(1,1452)	1:2:A:CYS:HB2	1:5:A:PRO:HA	4	0.19	0.05	0.2
(1,583)	1:26:A:THR:H	1:51:A:TRP:HH2	4	0.19	0.03	0.2
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG2	4	0.19	0.03	0.18
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG3	4	0.19	0.03	0.18
(1,2461)	1:90:A:CYS:HB2	1:91:A:THR:H	4	0.19	0.02	0.2
(1,2461)	1:90:A:CYS:HB3	1:91:A:THR:H	4	0.19	0.02	0.2
(1,1461)	1:4:A:ALA:H	1:20:A:PHE:HA	4	0.18	0.05	0.18
(1,88)	1:96:A:LEU:HD11	1:97:A:ILE:H	4	0.18	0.04	0.16
(1,88)	1:96:A:LEU:HD12	1:97:A:ILE:H	4	0.18	0.04	0.16
(1,88)	1:96:A:LEU:HD13	1:97:A:ILE:H	4	0.18	0.04	0.16
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD11	4	0.17	0.04	0.16
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD12	4	0.17	0.04	0.16
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD13	4	0.17	0.04	0.16
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD11	4	0.17	0.02	0.17
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD12	4	0.17	0.02	0.17
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD13	4	0.17	0.02	0.17
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD11	4	0.17	0.02	0.17
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD12	4	0.17	0.02	0.17
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD13	4	0.17	0.02	0.17
(1,1952)	1:36:A:TYR:HE1	1:61:A:LYS:H	4	0.17	0.08	0.13
(1,1952)	1:36:A:TYR:HE2	1:61:A:LYS:H	4	0.17	0.08	0.13
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE2	4	0.15	0.04	0.14
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE3	4	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1560)	1:5:A:PRO:HB2	1:6:A:GLU:HA	4	0.14	0.03	0.14
(1,2242)	1:60:A:ARG:HG2	1:81:A:GLN:HE21	4	0.14	0.04	0.12
(1,2242)	1:60:A:ARG:HG3	1:81:A:GLN:HE21	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD11	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD12	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD13	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD11	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD12	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD13	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD11	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD12	4	0.14	0.04	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD13	4	0.14	0.04	0.12
(1,914)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	4	0.13	0.03	0.12
(1,954)	1:68:A:ASP:H	1:69:A:PRO:HA	4	0.13	0.02	0.12
(1,447)	1:106:A:ILE:HG21	1:108:A:GLY:H	4	0.13	0.03	0.12
(1,447)	1:106:A:ILE:HG22	1:108:A:GLY:H	4	0.13	0.03	0.12
(1,447)	1:106:A:ILE:HG23	1:108:A:GLY:H	4	0.13	0.03	0.12
(1,141)	1:88:A:TYR:H	1:89:A:SER:H	4	0.12	0.0	0.12
(1,155)	1:92:A:LYS:H	1:93:A:GLY:H	3	0.8	0.19	0.74
(1,2252)	1:60:A:ARG:HD2	1:82:A:PHE:HA	3	0.51	0.14	0.55
(1,2252)	1:60:A:ARG:HD3	1:82:A:PHE:HA	3	0.51	0.14	0.55
(1,931)	1:65:A:ASN:HD22	1:67:A:PRO:HG2	3	0.46	0.15	0.54
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG2	3	0.43	0.11	0.46
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG3	3	0.43	0.11	0.46
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE1	3	0.43	0.37	0.22
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE2	3	0.43	0.37	0.22
(1,1814)	1:73:A:MET:HE1	1:92:A:LYS:H	3	0.41	0.16	0.42
(1,1814)	1:73:A:MET:HE2	1:92:A:LYS:H	3	0.41	0.16	0.42
(1,1814)	1:73:A:MET:HE3	1:92:A:LYS:H	3	0.41	0.16	0.42
(1,139)	1:80:A:ILE:H	1:81:A:GLN:H	3	0.4	0.18	0.48
(1,2116)	1:37:A:SER:HB2	1:38:A:GLY:H	3	0.39	0.1	0.34
(1,2116)	1:37:A:SER:HB3	1:38:A:GLY:H	3	0.39	0.1	0.34
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD1	3	0.31	0.12	0.25
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD2	3	0.31	0.12	0.25
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD1	3	0.31	0.12	0.25
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD2	3	0.31	0.12	0.25
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD1	3	0.31	0.12	0.25
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD2	3	0.31	0.12	0.25
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG2	3	0.3	0.08	0.35
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG3	3	0.3	0.08	0.35
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG2	3	0.3	0.08	0.35
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG3	3	0.3	0.08	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2363)	1:73:A:MET:HG2	1:90:A:CYS:HA	3	0.3	0.12	0.25
(1,2363)	1:73:A:MET:HG3	1:90:A:CYS:HA	3	0.3	0.12	0.25
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG2	3	0.3	0.13	0.36
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG3	3	0.3	0.13	0.36
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD11	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD12	3	0.3	0.1	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD13	3	0.3	0.1	0.33
(1,1525)	1:16:A:LEU:HB2	1:28:A:LEU:HG	3	0.28	0.17	0.2
(1,1525)	1:16:A:LEU:HB3	1:28:A:LEU:HG	3	0.28	0.17	0.2
(1,1553)	1:96:A:LEU:HD21	1:119:A:ILE:H	3	0.28	0.04	0.26
(1,1553)	1:96:A:LEU:HD22	1:119:A:ILE:H	3	0.28	0.04	0.26
(1,1553)	1:96:A:LEU:HD23	1:119:A:ILE:H	3	0.28	0.04	0.26
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB2	3	0.27	0.03	0.28
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB3	3	0.27	0.03	0.28
(1,1112)	1:33:A:ARG:H	1:36:A:TYR:HB3	3	0.26	0.15	0.21
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE1	3	0.26	0.18	0.13
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE2	3	0.26	0.18	0.13
(1,2428)	1:84:A:SER:HB2	1:104:A:CYS:H	3	0.26	0.03	0.24
(1,2428)	1:84:A:SER:HB3	1:104:A:CYS:H	3	0.26	0.03	0.24
(1,844)	1:28:A:LEU:HD11	1:29:A:ASN:H	3	0.25	0.12	0.19
(1,844)	1:28:A:LEU:HD12	1:29:A:ASN:H	3	0.25	0.12	0.19
(1,844)	1:28:A:LEU:HD13	1:29:A:ASN:H	3	0.25	0.12	0.19
(1,892)	1:3:A:ASN:HD21	1:4:A:ALA:H	3	0.25	0.11	0.25
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE1	3	0.25	0.08	0.2
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE2	3	0.25	0.08	0.2
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE3	3	0.25	0.08	0.2
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD2	3	0.24	0.15	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD2	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD2	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD2	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD2	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD2	3	0.24	0.15	0.16
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD3	3	0.24	0.15	0.16
(1,2283)	1:62:A:SER:HB2	1:64:A:ARG:HB3	3	0.24	0.03	0.23
(1,2283)	1:62:A:SER:HB3	1:64:A:ARG:HB3	3	0.24	0.03	0.23
(1,1217)	1:105:A:ILE:HD11	1:114:A:ASP:HB3	3	0.24	0.06	0.27
(1,1217)	1:105:A:ILE:HD12	1:114:A:ASP:HB3	3	0.24	0.06	0.27
(1,1217)	1:105:A:ILE:HD13	1:114:A:ASP:HB3	3	0.24	0.06	0.27
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB2	3	0.24	0.04	0.24
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB3	3	0.24	0.04	0.24
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE1	3	0.23	0.04	0.23
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE2	3	0.23	0.04	0.23
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG21	3	0.23	0.13	0.17
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG22	3	0.23	0.13	0.17
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG23	3	0.23	0.13	0.17
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD11	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD12	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD13	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD11	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD12	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD13	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD11	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD12	3	0.23	0.07	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD13	3	0.23	0.07	0.21
(1,637)	1:26:A:THR:HB	1:45:A:CYS:H	3	0.23	0.08	0.27
(1,667)	1:1:A:GLN:HB2	1:22:A:PHE:H	3	0.23	0.02	0.23
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB2	3	0.22	0.02	0.22
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB3	3	0.22	0.02	0.22
(1,2161)	1:47:A:LYS:HB2	1:52:A:THR:HA	3	0.22	0.09	0.21
(1,2161)	1:47:A:LYS:HB3	1:52:A:THR:HA	3	0.22	0.09	0.21
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG21	3	0.22	0.07	0.22
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG22	3	0.22	0.07	0.22
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG23	3	0.22	0.07	0.22
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG21	3	0.22	0.07	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG22	3	0.22	0.07	0.22
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG23	3	0.22	0.07	0.22
(1,1240)	1:4:A:ALA:HB1	1:51:A:TRP:HZ2	3	0.21	0.09	0.2
(1,1240)	1:4:A:ALA:HB2	1:51:A:TRP:HZ2	3	0.21	0.09	0.2
(1,1240)	1:4:A:ALA:HB3	1:51:A:TRP:HZ2	3	0.21	0.09	0.2
(1,1044)	1:2:A:CYS:HB2	1:51:A:TRP:HD1	3	0.21	0.07	0.19
(1,1123)	1:25:A:GLY:H	1:45:A:CYS:HA	3	0.21	0.05	0.2
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG11	3	0.2	0.04	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG12	3	0.2	0.04	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG13	3	0.2	0.04	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG11	3	0.2	0.04	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG12	3	0.2	0.04	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG13	3	0.2	0.04	0.23
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD1	3	0.2	0.03	0.21
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD2	3	0.2	0.03	0.21
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	3	0.2	0.08	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	3	0.2	0.08	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	3	0.2	0.08	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD21	3	0.2	0.08	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD22	3	0.2	0.08	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD23	3	0.2	0.08	0.19
(1,150)	1:92:A:LYS:HB2	1:93:A:GLY:H	3	0.19	0.06	0.19
(1,927)	1:65:A:ASN:HD21	1:68:A:ASP:HA	3	0.19	0.04	0.18
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA2	3	0.19	0.07	0.18
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA3	3	0.19	0.07	0.18
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA2	3	0.19	0.07	0.18
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA3	3	0.19	0.07	0.18
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA2	3	0.19	0.07	0.18
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA3	3	0.19	0.07	0.18
(1,183)	1:99:A:SER:H	1:119:A:ILE:H	3	0.18	0.04	0.16
(1,1889)	1:22:A:PHE:HB3	1:26:A:THR:HA	3	0.18	0.01	0.18
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD1	3	0.17	0.05	0.18
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD2	3	0.17	0.05	0.18
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE1	3	0.17	0.05	0.19
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE2	3	0.17	0.05	0.19
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE3	3	0.17	0.05	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE1	3	0.17	0.05	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE2	3	0.17	0.05	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE3	3	0.17	0.05	0.19
(1,120)	1:69:A:PRO:HB2	1:72:A:GLY:H	3	0.17	0.03	0.19
(1,864)	1:27:A:TYR:HE1	1:42:A:SER:H	3	0.17	0.02	0.18
(1,864)	1:27:A:TYR:HE2	1:42:A:SER:H	3	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD11	3	0.17	0.06	0.13
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD12	3	0.17	0.06	0.13
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD13	3	0.17	0.06	0.13
(1,1462)	1:96:A:LEU:HG	1:119:A:ILE:HB	3	0.17	0.05	0.14
(1,187)	1:88:A:TYR:HB2	1:119:A:ILE:H	3	0.15	0.01	0.16
(1,1231)	1:105:A:ILE:HG21	1:113:A:TRP:HE3	3	0.15	0.01	0.15
(1,1231)	1:105:A:ILE:HG22	1:113:A:TRP:HE3	3	0.15	0.01	0.15
(1,1231)	1:105:A:ILE:HG23	1:113:A:TRP:HE3	3	0.15	0.01	0.15
(1,1272)	1:14:A:THR:HG21	1:29:A:ASN:HB2	3	0.15	0.05	0.11
(1,1272)	1:14:A:THR:HG22	1:29:A:ASN:HB2	3	0.15	0.05	0.11
(1,1272)	1:14:A:THR:HG23	1:29:A:ASN:HB2	3	0.15	0.05	0.11
(1,228)	1:111:A:VAL:HG21	1:113:A:TRP:H	3	0.14	0.04	0.14
(1,228)	1:111:A:VAL:HG22	1:113:A:TRP:H	3	0.14	0.04	0.14
(1,228)	1:111:A:VAL:HG23	1:113:A:TRP:H	3	0.14	0.04	0.14
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB2	3	0.14	0.01	0.14
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB3	3	0.14	0.01	0.14
(1,401)	1:102:A:ALA:HA	1:115:A:GLN:H	3	0.13	0.01	0.14
(1,483)	1:98:A:GLY:HA2	1:100:A:SER:H	3	0.13	0.02	0.15
(1,781)	1:15:A:GLN:HB2	1:17:A:THR:H	3	0.13	0.01	0.12
(1,959)	1:22:A:PHE:H	1:51:A:TRP:HE1	3	0.13	0.02	0.12
(1,1318)	1:96:A:LEU:HD21	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,1318)	1:96:A:LEU:HD22	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,1318)	1:96:A:LEU:HD23	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD11	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD12	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD13	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD21	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD22	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,2507)	1:96:A:LEU:HD23	1:100:A:SER:HA	3	0.13	0.02	0.13
(1,377)	1:94:A:TYR:HE1	1:120:A:CYS:H	3	0.12	0.01	0.13
(1,377)	1:94:A:TYR:HE2	1:120:A:CYS:H	3	0.12	0.01	0.13
(1,926)	1:65:A:ASN:HA	1:65:A:ASN:HD21	3	0.12	0.03	0.11
(1,1340)	1:38:A:GLY:HA2	1:39:A:ARG:HB3	3	0.12	0.02	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD11	3	0.12	0.02	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD12	3	0.12	0.02	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD13	3	0.12	0.02	0.11
(1,1730)	1:85:A:GLN:HB2	1:113:A:TRP:HZ3	3	0.12	0.01	0.13
(1,2561)	1:109:A:ASP:HB2	1:110:A:THR:HB	3	0.12	0.0	0.12
(1,2561)	1:109:A:ASP:HB3	1:110:A:THR:HB	3	0.12	0.0	0.12
(1,1902)	1:24:A:ILE:HA	1:49:A:SER:HA	3	0.12	0.01	0.11
(1,565)	1:74:A:VAL:HB	1:87:A:LYS:H	3	0.12	0.01	0.11
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE2	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE3	3	0.12	0.0	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE2	3	0.12	0.0	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE3	3	0.12	0.0	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE2	3	0.12	0.0	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE3	3	0.12	0.0	0.12
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB2	2	0.66	0.14	0.66
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB3	2	0.66	0.14	0.66
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB2	2	0.66	0.14	0.66
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB3	2	0.66	0.14	0.66
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD11	2	0.64	0.04	0.64
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD12	2	0.64	0.04	0.64
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD13	2	0.64	0.04	0.64
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG2	2	0.59	0.03	0.59
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG3	2	0.59	0.03	0.59
(1,847)	1:38:A:GLY:HA2	1:39:A:ARG:H	2	0.54	0.13	0.54
(1,646)	1:76:A:VAL:H	1:76:A:VAL:HB	2	0.5	0.02	0.5
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG11	2	0.46	0.01	0.46
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG12	2	0.46	0.01	0.46
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG13	2	0.46	0.01	0.46
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD2	2	0.44	0.01	0.44
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD3	2	0.44	0.01	0.44
(1,861)	1:41:A:PHE:HA	1:42:A:SER:H	2	0.42	0.01	0.42
(1,2289)	1:63:A:CYS:HB2	1:81:A:GLN:H	2	0.42	0.26	0.42
(1,2289)	1:63:A:CYS:HB3	1:81:A:GLN:H	2	0.42	0.26	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD11	2	0.42	0.02	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD12	2	0.42	0.02	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD13	2	0.42	0.02	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD21	2	0.42	0.02	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD22	2	0.42	0.02	0.42
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD23	2	0.42	0.02	0.42
(1,2297)	1:63:A:CYS:HB2	1:113:A:TRP:HE1	2	0.38	0.24	0.38
(1,2297)	1:63:A:CYS:HB3	1:113:A:TRP:HE1	2	0.38	0.24	0.38
(1,760)	1:50:A:VAL:H	1:51:A:TRP:H	2	0.38	0.04	0.38
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG2	2	0.37	0.01	0.37
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG3	2	0.37	0.01	0.37
(1,157)	1:37:A:SER:H	1:38:A:GLY:H	2	0.36	0.05	0.36
(1,960)	1:51:A:TRP:H	1:51:A:TRP:HD1	2	0.35	0.03	0.35
(1,780)	1:17:A:THR:H	1:19:A:GLU:HG3	2	0.34	0.13	0.34
(1,2015)	1:8:A:LEU:HD11	1:9:A:PRO:HD3	2	0.34	0.06	0.34
(1,2015)	1:8:A:LEU:HD12	1:9:A:PRO:HD3	2	0.34	0.06	0.34
(1,2015)	1:8:A:LEU:HD13	1:9:A:PRO:HD3	2	0.34	0.06	0.34
(1,2015)	1:8:A:LEU:HD21	1:9:A:PRO:HD3	2	0.34	0.06	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2015)	1:8:A:LEU:HD22	1:9:A:PRO:HD3	2	0.34	0.06	0.34
(1,2015)	1:8:A:LEU:HD23	1:9:A:PRO:HD3	2	0.34	0.06	0.34
(1,2388)	1:76:A:VAL:HG11	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2388)	1:76:A:VAL:HG12	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2388)	1:76:A:VAL:HG13	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2388)	1:76:A:VAL:HG21	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2388)	1:76:A:VAL:HG22	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2388)	1:76:A:VAL:HG23	1:78:A:LYS:H	2	0.34	0.13	0.34
(1,2166)	1:47:A:LYS:HG2	1:50:A:VAL:H	2	0.32	0.02	0.32
(1,2166)	1:47:A:LYS:HG3	1:50:A:VAL:H	2	0.32	0.02	0.32
(1,2481)	1:92:A:LYS:HE2	1:93:A:GLY:H	2	0.32	0.05	0.32
(1,2481)	1:92:A:LYS:HE3	1:93:A:GLY:H	2	0.32	0.05	0.32
(1,1295)	1:92:A:LYS:H	1:92:A:LYS:HB2	2	0.31	0.02	0.31
(1,923)	1:15:A:GLN:HE21	1:28:A:LEU:HG	2	0.3	0.15	0.3
(1,2267)	1:61:A:LYS:HG2	1:62:A:SER:HA	2	0.3	0.04	0.3
(1,2267)	1:61:A:LYS:HG3	1:62:A:SER:HA	2	0.3	0.04	0.3
(1,1325)	1:60:A:ARG:H	1:60:A:ARG:HD2	2	0.29	0.02	0.29
(1,133)	1:79:A:GLY:H	1:80:A:ILE:H	2	0.29	0.14	0.29
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE1	2	0.29	0.05	0.29
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE2	2	0.29	0.05	0.29
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE3	2	0.29	0.05	0.29
(1,81)	1:60:A:ARG:H	1:60:A:ARG:HD3	2	0.28	0.09	0.28
(1,649)	1:74:A:VAL:H	1:89:A:SER:H	2	0.27	0.03	0.27
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD1	2	0.27	0.03	0.27
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD2	2	0.27	0.03	0.27
(1,2027)	1:8:A:LEU:HD11	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,2027)	1:8:A:LEU:HD12	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,2027)	1:8:A:LEU:HD13	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,2027)	1:8:A:LEU:HD21	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,2027)	1:8:A:LEU:HD22	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,2027)	1:8:A:LEU:HD23	1:54:A:ALA:HA	2	0.27	0.01	0.27
(1,692)	1:61:A:LYS:H	1:81:A:GLN:HE21	2	0.26	0.16	0.26
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB2	2	0.26	0.03	0.26
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB3	2	0.26	0.03	0.26
(1,48)	1:12:A:ARG:H	1:32:A:CYS:H	2	0.25	0.08	0.25
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG21	2	0.25	0.08	0.25
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG22	2	0.25	0.08	0.25
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG23	2	0.25	0.08	0.25
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG2	2	0.25	0.03	0.25
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG3	2	0.25	0.03	0.25
(1,495)	1:96:A:LEU:H	1:120:A:CYS:HA	2	0.24	0.02	0.24
(1,1750)	1:8:A:LEU:HG	1:10:A:PHE:HB3	2	0.24	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB2	2	0.24	0.04	0.24
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB3	2	0.24	0.04	0.24
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD1	2	0.24	0.05	0.24
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD2	2	0.24	0.05	0.24
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG11	2	0.24	0.06	0.24
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG12	2	0.24	0.06	0.24
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG13	2	0.24	0.06	0.24
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG11	2	0.24	0.06	0.24
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG12	2	0.24	0.06	0.24
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG13	2	0.24	0.06	0.24
(1,360)	1:105:A:ILE:H	1:114:A:ASP:HA	2	0.23	0.03	0.23
(1,415)	1:55:A:LYS:HA	1:57:A:ARG:H	2	0.23	0.03	0.23
(1,2209)	1:55:A:LYS:HG2	1:56:A:ASP:HA	2	0.23	0.01	0.23
(1,2209)	1:55:A:LYS:HG3	1:56:A:ASP:HA	2	0.23	0.01	0.23
(1,180)	1:38:A:GLY:HA3	1:58:A:CYS:H	2	0.22	0.08	0.22
(1,1763)	1:16:A:LEU:HA	1:20:A:PHE:HB2	2	0.22	0.02	0.22
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD11	2	0.22	0.05	0.22
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD12	2	0.22	0.05	0.22
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD13	2	0.22	0.05	0.22
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD11	2	0.22	0.05	0.22
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD12	2	0.22	0.05	0.22
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD13	2	0.22	0.05	0.22
(1,1463)	1:96:A:LEU:HG	1:119:A:ILE:H	2	0.22	0.04	0.22
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG2	2	0.22	0.07	0.22
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG3	2	0.22	0.07	0.22
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD11	2	0.22	0.07	0.22
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD12	2	0.22	0.07	0.22
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD13	2	0.22	0.07	0.22
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG11	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG12	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG13	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG21	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)
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG22	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG23	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG11	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG12	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG13	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG21	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG22	2	0.22	0.1	0.22
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG23	2	0.22	0.1	0.22
(1,2478)	1:92:A:LYS:HD2	1:93:A:GLY:H	2	0.22	0.1	0.22
(1,2478)	1:92:A:LYS:HD3	1:93:A:GLY:H	2	0.22	0.1	0.22
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD11	2	0.21	0.1	0.21
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD12	2	0.21	0.1	0.21
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD13	2	0.21	0.1	0.21
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD11	2	0.21	0.1	0.21
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD12	2	0.21	0.1	0.21
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD13	2	0.21	0.1	0.21
(1,2556)	1:107:A:SER:HB2	1:112:A:ILE:H	2	0.21	0.0	0.21
(1,2556)	1:107:A:SER:HB3	1:112:A:ILE:H	2	0.21	0.0	0.21
(1,83)	1:36:A:TYR:HE1	1:60:A:ARG:H	2	0.2	0.0	0.2
(1,83)	1:36:A:TYR:HE2	1:60:A:ARG:H	2	0.2	0.0	0.2
(1,905)	1:1:A:GLN:HB2	1:1:A:GLN:HE22	2	0.2	0.0	0.2
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG2	2	0.2	0.03	0.2
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG3	2	0.2	0.03	0.2
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD2	2	0.2	0.0	0.2
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD3	2	0.2	0.0	0.2
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD2	2	0.2	0.0	0.2
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD3	2	0.2	0.0	0.2
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB2	2	0.2	0.04	0.2
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB3	2	0.2	0.04	0.2
(1,747)	1:24:A:ILE:H	1:24:A:ILE:HG12	2	0.2	0.09	0.2
(1,943)	1:46:A:LEU:H	1:51:A:TRP:H	2	0.2	0.08	0.2
(1,1479)	1:110:A:THR:HG21	1:112:A:ILE:HB	2	0.2	0.04	0.2
(1,1479)	1:110:A:THR:HG22	1:112:A:ILE:HB	2	0.2	0.04	0.2
(1,1479)	1:110:A:THR:HG23	1:112:A:ILE:HB	2	0.2	0.04	0.2
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD11	2	0.2	0.06	0.2
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD12	2	0.2	0.06	0.2
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD13	2	0.2	0.06	0.2
(1,2395)	1:76:A:VAL:HG11	1:113:A:TRP:HZ2	2	0.2	0.05	0.2
(1,2395)	1:76:A:VAL:HG12	1:113:A:TRP:HZ2	2	0.2	0.05	0.2
(1,2395)	1:76:A:VAL:HG13	1:113:A:TRP:HZ2	2	0.2	0.05	0.2
(1,2395)	1:76:A:VAL:HG21	1:113:A:TRP:HZ2	2	0.2	0.05	0.2
(1,2395)	1:76:A:VAL:HG22	1:113:A:TRP:HZ2	2	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2395)	1:76:A:VAL:HG23	1:113:A:TRP:HZ2	2	0.2	0.05	0.2
(1,1040)	1:95:A:ARG:HB2	1:121:A:ASP:HB3	2	0.19	0.08	0.19
(1,23)	1:36:A:TYR:HE1	1:37:A:SER:H	2	0.18	0.01	0.18
(1,23)	1:36:A:TYR:HE2	1:37:A:SER:H	2	0.18	0.01	0.18
(1,757)	1:24:A:ILE:HG13	1:49:A:SER:H	2	0.18	0.01	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD11	2	0.18	0.01	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD12	2	0.18	0.01	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD13	2	0.18	0.01	0.18
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB2	2	0.18	0.04	0.18
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB3	2	0.18	0.04	0.18
(1,1574)	1:87:A:LYS:HA	1:100:A:SER:HA	2	0.18	0.01	0.18
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG21	2	0.18	0.05	0.18
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG22	2	0.18	0.05	0.18
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG23	2	0.18	0.05	0.18
(1,1898)	1:15:A:GLN:HB3	1:15:A:GLN:HE22	2	0.18	0.02	0.18
(1,1242)	1:3:A:ASN:H	1:51:A:TRP:HZ2	2	0.18	0.02	0.18
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD1	2	0.18	0.08	0.18
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD2	2	0.18	0.08	0.18
(1,786)	1:15:A:GLN:HB2	1:16:A:LEU:H	2	0.17	0.03	0.17
(1,893)	1:3:A:ASN:HA	1:3:A:ASN:HD21	2	0.17	0.01	0.17
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG21	2	0.17	0.02	0.17
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG22	2	0.17	0.02	0.17
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG23	2	0.17	0.02	0.17
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG21	2	0.16	0.02	0.16
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG22	2	0.16	0.02	0.16
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG23	2	0.16	0.02	0.16
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG2	2	0.16	0.01	0.16
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG3	2	0.16	0.01	0.16
(1,1697)	1:99:A:SER:HB3	1:115:A:GLN:HA	2	0.16	0.04	0.16
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG11	2	0.16	0.04	0.16
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG12	2	0.16	0.04	0.16
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG13	2	0.16	0.04	0.16
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB1	2	0.16	0.05	0.16
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB2	2	0.16	0.05	0.16
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB3	2	0.16	0.05	0.16
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB1	2	0.16	0.05	0.16
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB2	2	0.16	0.05	0.16
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB3	2	0.16	0.05	0.16
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG21	2	0.16	0.05	0.16
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG22	2	0.16	0.05	0.16
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG23	2	0.16	0.05	0.16
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD2	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD3	2	0.16	0.04	0.16
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD2	2	0.16	0.04	0.16
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD3	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG11	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG12	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG13	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG21	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG22	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,2387)	1:76:A:VAL:HG23	1:77:A:ILE:H	2	0.16	0.04	0.16
(1,425)	1:102:A:ALA:HB1	1:116:A:GLU:H	2	0.16	0.02	0.16
(1,425)	1:102:A:ALA:HB2	1:116:A:GLU:H	2	0.16	0.02	0.16
(1,425)	1:102:A:ALA:HB3	1:116:A:GLU:H	2	0.16	0.02	0.16
(1,290)	1:86:A:ILE:HD11	1:104:A:CYS:H	2	0.16	0.05	0.16
(1,290)	1:86:A:ILE:HD12	1:104:A:CYS:H	2	0.16	0.05	0.16
(1,290)	1:86:A:ILE:HD13	1:104:A:CYS:H	2	0.16	0.05	0.16
(1,887)	1:4:A:ALA:HB1	1:51:A:TRP:HE1	2	0.16	0.02	0.16
(1,887)	1:4:A:ALA:HB2	1:51:A:TRP:HE1	2	0.16	0.02	0.16
(1,887)	1:4:A:ALA:HB3	1:51:A:TRP:HE1	2	0.16	0.02	0.16
(1,898)	1:1:A:GLN:H	1:1:A:GLN:HE22	2	0.16	0.01	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG11	2	0.16	0.05	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG12	2	0.16	0.05	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG13	2	0.16	0.05	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG21	2	0.16	0.05	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG22	2	0.16	0.05	0.16
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG23	2	0.16	0.05	0.16
(1,156)	1:93:A:GLY:H	1:94:A:TYR:H	2	0.15	0.02	0.15
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG21	2	0.15	0.02	0.15
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG22	2	0.15	0.02	0.15
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG23	2	0.15	0.02	0.15
(1,1700)	1:5:A:PRO:HD2	1:20:A:PHE:HB3	2	0.15	0.05	0.15
(1,639)	1:45:A:CYS:H	1:51:A:TRP:HB3	2	0.15	0.03	0.15
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD1	2	0.15	0.02	0.15
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD2	2	0.15	0.02	0.15
(1,2056)	1:16:A:LEU:HD11	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,2056)	1:16:A:LEU:HD12	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,2056)	1:16:A:LEU:HD13	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,2056)	1:16:A:LEU:HD21	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,2056)	1:16:A:LEU:HD22	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,2056)	1:16:A:LEU:HD23	1:17:A:THR:HB	2	0.15	0.03	0.15
(1,1144)	1:10:A:PHE:HA	1:58:A:CYS:HB3	2	0.14	0.01	0.14
(1,1439)	1:44:A:ILE:HD11	1:51:A:TRP:HA	2	0.14	0.03	0.14
(1,1439)	1:44:A:ILE:HD12	1:51:A:TRP:HA	2	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1439)	1:44:A:ILE:HD13	1:51:A:TRP:HA	2	0.14	0.03	0.14
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD11	2	0.14	0.03	0.14
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD12	2	0.14	0.03	0.14
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD13	2	0.14	0.03	0.14
(1,1959)	1:43:A:ILE:HB	1:51:A:TRP:HD1	2	0.14	0.01	0.14
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB2	2	0.14	0.03	0.14
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB3	2	0.14	0.03	0.14
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA2	2	0.14	0.02	0.14
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA3	2	0.14	0.02	0.14
(1,273)	1:10:A:PHE:HD1	1:33:A:ARG:H	2	0.14	0.02	0.14
(1,273)	1:10:A:PHE:HD2	1:33:A:ARG:H	2	0.14	0.02	0.14
(1,1535)	1:105:A:ILE:HD11	1:115:A:GLN:H	2	0.14	0.01	0.14
(1,1535)	1:105:A:ILE:HD12	1:115:A:GLN:H	2	0.14	0.01	0.14
(1,1535)	1:105:A:ILE:HD13	1:115:A:GLN:H	2	0.14	0.01	0.14
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG2	2	0.14	0.02	0.14
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG3	2	0.14	0.02	0.14
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD11	2	0.13	0.02	0.13
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD12	2	0.13	0.02	0.13
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD13	2	0.13	0.02	0.13
(1,808)	1:4:A:ALA:HA	1:20:A:PHE:H	2	0.13	0.02	0.13
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG11	2	0.13	0.02	0.13
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG12	2	0.13	0.02	0.13
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG13	2	0.13	0.02	0.13
(1,1283)	1:24:A:ILE:HD11	1:25:A:GLY:H	2	0.13	0.01	0.13
(1,1283)	1:24:A:ILE:HD12	1:25:A:GLY:H	2	0.13	0.01	0.13
(1,1283)	1:24:A:ILE:HD13	1:25:A:GLY:H	2	0.13	0.01	0.13
(1,1486)	1:44:A:ILE:HD11	1:52:A:THR:HA	2	0.13	0.01	0.13
(1,1486)	1:44:A:ILE:HD12	1:52:A:THR:HA	2	0.13	0.01	0.13
(1,1486)	1:44:A:ILE:HD13	1:52:A:THR:HA	2	0.13	0.01	0.13
(1,939)	1:81:A:GLN:HB2	1:81:A:GLN:HE21	2	0.12	0.02	0.12
(1,1269)	1:14:A:THR:HG21	1:29:A:ASN:H	2	0.12	0.02	0.12
(1,1269)	1:14:A:THR:HG22	1:29:A:ASN:H	2	0.12	0.02	0.12
(1,1269)	1:14:A:THR:HG23	1:29:A:ASN:H	2	0.12	0.02	0.12
(1,1759)	1:106:A:ILE:HB	1:107:A:SER:HA	2	0.12	0.01	0.12
(1,2221)	1:57:A:ARG:HG2	1:58:A:CYS:H	2	0.12	0.02	0.12
(1,2221)	1:57:A:ARG:HG3	1:58:A:CYS:H	2	0.12	0.02	0.12
(1,1219)	1:117:A:THR:HG21	1:119:A:ILE:HA	2	0.12	0.02	0.12
(1,1219)	1:117:A:THR:HG22	1:119:A:ILE:HA	2	0.12	0.02	0.12
(1,1219)	1:117:A:THR:HG23	1:119:A:ILE:HA	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG21	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG22	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG23	2	0.12	0.02	0.12

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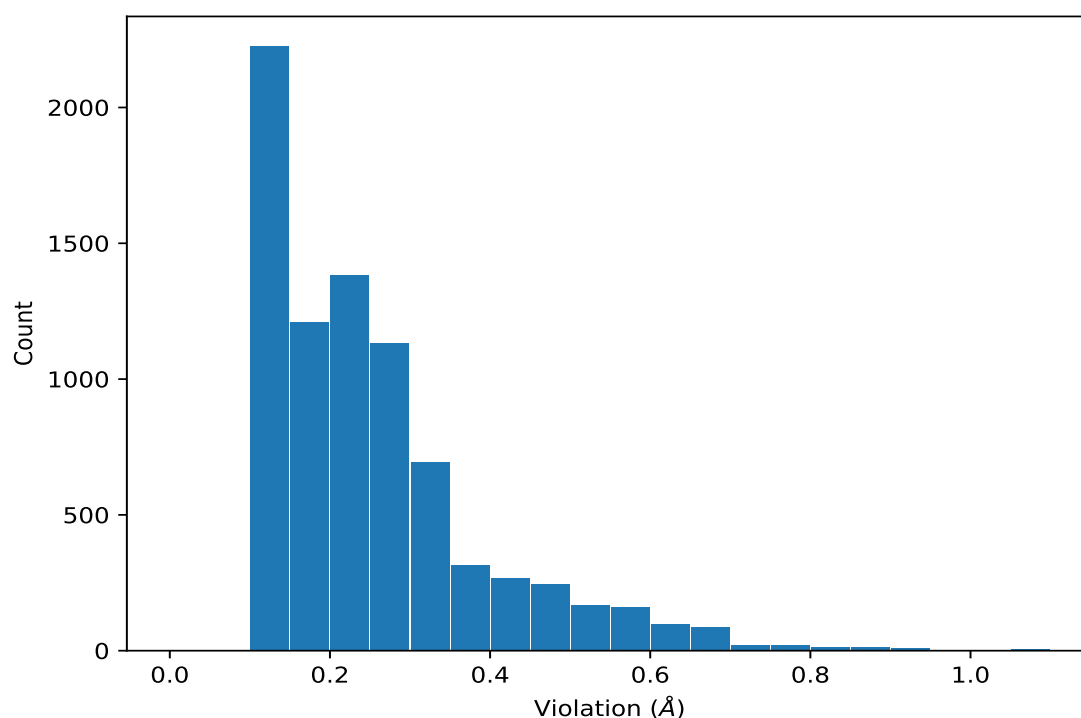
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG21	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG22	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG23	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG21	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG22	2	0.12	0.02	0.12
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG23	2	0.12	0.02	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE1	2	0.12	0.0	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE2	2	0.12	0.0	0.12
(1,1453)	1:63:A:CYS:HA	1:64:A:ARG:HB3	2	0.12	0.01	0.12
(1,1947)	1:36:A:TYR:HE1	1:59:A:ARG:HA	2	0.12	0.01	0.12
(1,1947)	1:36:A:TYR:HE2	1:59:A:ARG:HA	2	0.12	0.01	0.12
(1,123)	1:8:A:LEU:HD21	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,123)	1:8:A:LEU:HD22	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,123)	1:8:A:LEU:HD23	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,181)	1:10:A:PHE:HE1	1:58:A:CYS:H	2	0.12	0.0	0.12
(1,181)	1:10:A:PHE:HE2	1:58:A:CYS:H	2	0.12	0.0	0.12
(1,254)	1:14:A:THR:HA	1:15:A:GLN:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD11	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD12	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD13	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD21	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD22	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2016)	1:8:A:LEU:HD23	1:10:A:PHE:H	2	0.12	0.0	0.12
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB2	2	0.12	0.0	0.12
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB3	2	0.12	0.0	0.12
(1,591)	1:84:A:SER:H	1:104:A:CYS:H	2	0.11	0.0	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG21	2	0.11	0.0	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG22	2	0.11	0.0	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG23	2	0.11	0.0	0.11
(1,1925)	1:8:A:LEU:HD21	1:9:A:PRO:HG2	2	0.11	0.0	0.11
(1,1925)	1:8:A:LEU:HD22	1:9:A:PRO:HG2	2	0.11	0.0	0.11
(1,1925)	1:8:A:LEU:HD23	1:9:A:PRO:HG2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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)
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	4	1.06
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	4	1.06
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	4	1.06
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	14	1.05
(1,155)	1:92:A:LYS:H	1:93:A:GLY:H	9	1.05
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	3	0.99
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE1	20	0.95
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE2	20	0.95
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	7	0.95
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	7	0.95
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	7	0.95
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	8	0.94
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	8	0.94
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	9	0.93
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	9	0.93
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	2	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	2	0.92
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	5	0.89
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	5	0.89
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	5	0.89
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	1	0.87
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	6	0.87
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	6	0.87
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	6	0.87
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	18	0.87
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	4	0.86
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	4	0.86
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	8	0.86
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	8	0.86
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	7	0.86
(1,533)	1:89:A:SER:HA	1:91:A:THR:H	17	0.84
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	8	0.83
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	13	0.83
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	13	0.83
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	20	0.83
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	4	0.82
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	4	0.82
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	17	0.8
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	17	0.8
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	17	0.8
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	17	0.8
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	19	0.8
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	7	0.8
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB2	11	0.79
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB3	11	0.79
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB2	11	0.79
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB3	11	0.79
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	19	0.79
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	14	0.78
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	14	0.78
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	14	0.78
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	14	0.78
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	11	0.78
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	10	0.77
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	10	0.77
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	20	0.77
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	20	0.77
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	11	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	8	0.76
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	8	0.76
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	14	0.76
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	5	0.76
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	3	0.75
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	3	0.75
(1,533)	1:89:A:SER:HA	1:91:A:THR:H	9	0.75
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	20	0.74
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	20	0.74
(1,155)	1:92:A:LYS:H	1:93:A:GLY:H	6	0.74
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	13	0.73
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	13	0.73
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG2	6	0.73
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG3	6	0.73
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	13	0.73
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	13	0.73
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	20	0.73
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG2	18	0.72
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG3	18	0.72
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	4	0.72
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	17	0.72
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	16	0.72
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	16	0.72
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	16	0.72
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	12	0.72
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	12	0.72
(1,533)	1:89:A:SER:HA	1:91:A:THR:H	13	0.72
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	12	0.72
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	1	0.71
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	6	0.7
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	6	0.7
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	14	0.7
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	14	0.7
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	10	0.7
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	10	0.7
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	6	0.7
(1,2289)	1:63:A:CYS:HB2	1:81:A:GLN:H	17	0.69
(1,2289)	1:63:A:CYS:HB3	1:81:A:GLN:H	17	0.69
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	11	0.69
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	11	0.69
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	14	0.69
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	14	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	17	0.69
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	17	0.69
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	17	0.69
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	17	0.69
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	17	0.69
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	17	0.69
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	9	0.69
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	9	0.69
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	8	0.69
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	1	0.69
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	1	0.69
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	1	0.69
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	1	0.69
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	1	0.69
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	1	0.69
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	11	0.69
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	5	0.69
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	6	0.68
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	6	0.68
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	19	0.68
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	19	0.68
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	20	0.68
(1,716)	1:5:A:PRO:HD2	1:6:A:GLU:H	8	0.68
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD11	15	0.68
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD12	15	0.68
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD13	15	0.68
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	10	0.68
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	15	0.67
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	15	0.67
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	15	0.67
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	15	0.67
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	19	0.67
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	19	0.67
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	19	0.67
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	19	0.67
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	12	0.67
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	8	0.67
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	8	0.67
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	8	0.67
(1,847)	1:38:A:GLY:HA2	1:39:A:ARG:H	2	0.67
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	1	0.66
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	19	0.66
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	19	0.66
(1,2252)	1:60:A:ARG:HD2	1:82:A:PHE:HA	6	0.66
(1,2252)	1:60:A:ARG:HD3	1:82:A:PHE:HA	6	0.66
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	1	0.66
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	1	0.66
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	7	0.66
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	7	0.66
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	9	0.66
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	9	0.66
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	11	0.66
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	2	0.66
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	18	0.66
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	5	0.65
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	5	0.65
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	13	0.65
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	13	0.65
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	1	0.65
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	1	0.65
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	2	0.65
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	2	0.65
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	20	0.65
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	20	0.65
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	20	0.65
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	20	0.65
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	20	0.65
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	20	0.65
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	7	0.65
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	20	0.65
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	3	0.65
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	19	0.65
(1,735)	1:44:A:ILE:H	1:52:A:THR:H	12	0.65
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	8	0.64
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	8	0.64
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	14	0.64
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	14	0.64
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	14	0.64
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	14	0.64
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	18	0.64
(1,554)	1:87:A:LYS:HG3	1:88:A:TYR:H	8	0.64
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	9	0.64
(1,2297)	1:63:A:CYS:HB2	1:113:A:TRP:HE1	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2297)	1:63:A:CYS:HB3	1:113:A:TRP:HE1	17	0.63
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	10	0.63
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	10	0.63
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE2	15	0.63
(1,2197)	1:55:A:LYS:H	1:55:A:LYS:HE3	15	0.63
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	18	0.63
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	18	0.63
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	18	0.63
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	18	0.63
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	18	0.63
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	18	0.63
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	10	0.63
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	16	0.63
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	16	0.63
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	19	0.63
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	19	0.63
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	19	0.63
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	11	0.62
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	11	0.62
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG2	10	0.62
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG3	10	0.62
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	3	0.62
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	3	0.62
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	17	0.62
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	17	0.62
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	2	0.62
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	2	0.62
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	8	0.62
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	8	0.62
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	8	0.62
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	8	0.62
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	3	0.62
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	19	0.62
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	19	0.62
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	19	0.62
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	14	0.62
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	10	0.62
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	16	0.62
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	20	0.62
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	20	0.62
(1,554)	1:87:A:LYS:HG3	1:88:A:TYR:H	10	0.62
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	20	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	20	0.62
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	20	0.62
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	1	0.61
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	1	0.61
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	10	0.61
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	10	0.61
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	18	0.61
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	18	0.61
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	18	0.61
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	18	0.61
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	19	0.61
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	19	0.61
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	9	0.61
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	9	0.61
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	9	0.61
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	9	0.61
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	12	0.61
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	12	0.61
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	3	0.61
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	3	0.61
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	3	0.61
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	3	0.61
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	3	0.61
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	3	0.61
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	13	0.61
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	13	0.61
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	13	0.61
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	13	0.61
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	13	0.61
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	13	0.61
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	19	0.61
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	19	0.61
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	3	0.61
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	13	0.61
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	15	0.61
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	16	0.61
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	5	0.61
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	5	0.61
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD11	3	0.61
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD12	3	0.61
(1,530)	1:96:A:LEU:H	1:97:A:ILE:HD13	3	0.61
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	1	0.61
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	1	0.61
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	1	0.61
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	10	0.61
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	8	0.6
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	8	0.6
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	8	0.6
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	8	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	6	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	6	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	7	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	7	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	19	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	19	0.6
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	7	0.6
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	7	0.6
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	7	0.6
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	7	0.6
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	4	0.6
(1,1814)	1:73:A:MET:HE1	1:92:A:LYS:H	17	0.6
(1,1814)	1:73:A:MET:HE2	1:92:A:LYS:H	17	0.6
(1,1814)	1:73:A:MET:HE3	1:92:A:LYS:H	17	0.6
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	11	0.6
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	11	0.6
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	11	0.6
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	11	0.6
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	11	0.6
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	11	0.6
(1,155)	1:92:A:LYS:H	1:93:A:GLY:H	15	0.6
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	14	0.59
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	14	0.59
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	15	0.59
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	15	0.59
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	4	0.59
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	4	0.59
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	13	0.59
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	13	0.59
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	13	0.59
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	13	0.59
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	6	0.59
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	15	0.59
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	14	0.59
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	11	0.59
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	11	0.59
(1,931)	1:65:A:ASN:HD22	1:67:A:PRO:HG2	18	0.59
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	3	0.58
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	3	0.58
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	16	0.58
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	16	0.58
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	6	0.58
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	6	0.58
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	9	0.58
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	9	0.58
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	16	0.58
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	16	0.58
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	16	0.58
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	16	0.58
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	16	0.58
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	16	0.58
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	18	0.58
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	11	0.58
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	3	0.58
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	9	0.58
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	9	0.58
(1,554)	1:87:A:LYS:HG3	1:88:A:TYR:H	4	0.58
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	6	0.58
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	20	0.58
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	9	0.57
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	9	0.57
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	9	0.57
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	9	0.57
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	12	0.57
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	12	0.57
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	18	0.57
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	18	0.57
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	3	0.57
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	3	0.57
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	7	0.57
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	7	0.57
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	8	0.57
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	17	0.57
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	18	0.57
(1,1528)	1:15:A:GLN:HB2	1:28:A:LEU:HG	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	12	0.57
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	1	0.57
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	1	0.57
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	1	0.57
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	14	0.57
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	3	0.57
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	8	0.57
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	5	0.57
(1,139)	1:80:A:ILE:H	1:81:A:GLN:H	12	0.57
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG2	7	0.56
(1,2488)	1:95:A:ARG:H	1:95:A:ARG:HG3	7	0.56
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	11	0.56
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	11	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	16	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	16	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	16	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	16	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	16	0.56
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	16	0.56
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	16	0.56
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	12	0.56
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	12	0.56
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	12	0.56
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	12	0.56
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	6	0.56
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	2	0.56
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	4	0.56
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	4	0.56
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	5	0.56
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	5	0.56
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	19	0.56
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	14	0.56
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	20	0.56
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	7	0.56
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	7	0.56
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	7	0.56
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	15	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:74:A:VAL:HG11	1:89:A:SER:H	13	0.56
(1,148)	1:74:A:VAL:HG12	1:89:A:SER:H	13	0.56
(1,148)	1:74:A:VAL:HG13	1:89:A:SER:H	13	0.56
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	5	0.55
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	5	0.55
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	20	0.55
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	20	0.55
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG2	9	0.55
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG3	9	0.55
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	6	0.55
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	6	0.55
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	6	0.55
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	6	0.55
(1,2252)	1:60:A:ARG:HD2	1:82:A:PHE:HA	17	0.55
(1,2252)	1:60:A:ARG:HD3	1:82:A:PHE:HA	17	0.55
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	17	0.55
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	17	0.55
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	1	0.55
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	1	0.55
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	14	0.55
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	14	0.55
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	1	0.55
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	1	0.55
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB2	6	0.55
(1,1658)	1:16:A:LEU:HA	1:19:A:GLU:HB3	6	0.55
(1,1499)	1:58:A:CYS:HA	1:59:A:ARG:HD3	4	0.55
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	6	0.55
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	6	0.55
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	4	0.55
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	19	0.55
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	11	0.55
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	12	0.55
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	16	0.55
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	16	0.55
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	16	0.55
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	3	0.55
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	3	0.55
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	3	0.55
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	19	0.54
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	19	0.54
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	7	0.54
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	7	0.54
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	7	0.54
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	7	0.54
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	1	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	7	0.54
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	7	0.54
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	2	0.54
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	13	0.54
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	7	0.54
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	7	0.54
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	7	0.54
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	7	0.54
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	7	0.54
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	7	0.54
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	3	0.54
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	7	0.54
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	9	0.54
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	13	0.54
(1,931)	1:65:A:ASN:HD22	1:67:A:PRO:HG2	2	0.54
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	20	0.54
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	1	0.54
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	4	0.54
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	19	0.54
(1,554)	1:87:A:LYS:HG3	1:88:A:TYR:H	3	0.54
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	16	0.54
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	1	0.54
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	18	0.54
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	18	0.54
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	18	0.54
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	7	0.53
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	7	0.53
(1,2164)	1:47:A:LYS:HG2	1:48:A:ASN:HB2	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2164)	1:47:A:LYS:HG2	1:48:A:ASN:HB3	1	0.53
(1,2164)	1:47:A:LYS:HG3	1:48:A:ASN:HB2	1	0.53
(1,2164)	1:47:A:LYS:HG3	1:48:A:ASN:HB3	1	0.53
(1,2116)	1:37:A:SER:HB2	1:38:A:GLY:H	1	0.53
(1,2116)	1:37:A:SER:HB3	1:38:A:GLY:H	1	0.53
(1,1989)	1:4:A:ALA:HB1	1:21:A:GLU:HG2	3	0.53
(1,1989)	1:4:A:ALA:HB1	1:21:A:GLU:HG3	3	0.53
(1,1989)	1:4:A:ALA:HB2	1:21:A:GLU:HG2	3	0.53
(1,1989)	1:4:A:ALA:HB2	1:21:A:GLU:HG3	3	0.53
(1,1989)	1:4:A:ALA:HB3	1:21:A:GLU:HG2	3	0.53
(1,1989)	1:4:A:ALA:HB3	1:21:A:GLU:HG3	3	0.53
(1,1524)	1:13:A:PRO:HA	1:14:A:THR:HB	4	0.53
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	7	0.53
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	9	0.53
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	15	0.53
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	10	0.53
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	6	0.53
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	4	0.53
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	4	0.53
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	4	0.53
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	16	0.52
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	16	0.52
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	16	0.52
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	16	0.52
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	16	0.52
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	16	0.52
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB2	10	0.52
(1,2268)	1:61:A:LYS:HG2	1:62:A:SER:HB3	10	0.52
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB2	10	0.52
(1,2268)	1:61:A:LYS:HG3	1:62:A:SER:HB3	10	0.52
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	1	0.52
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	1	0.52
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	5	0.52
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	5	0.52
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	10	0.52
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	10	0.52
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	20	0.52
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	20	0.52
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	20	0.52
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	20	0.52
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	0.52
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	17	0.52
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	17	0.52
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	17	0.52
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	17	0.52
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	17	0.52
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	17	0.52
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	17	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	19	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	19	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	19	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	19	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	19	0.52
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	19	0.52
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	12	0.52
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	18	0.52
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	18	0.52
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	18	0.52
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	18	0.52
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	18	0.52
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	18	0.52
(1,1525)	1:16:A:LEU:HB2	1:28:A:LEU:HG	20	0.52
(1,1525)	1:16:A:LEU:HB3	1:28:A:LEU:HG	20	0.52
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	9	0.52
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	9	0.52
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	9	0.52
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	8	0.52
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	8	0.52
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	2	0.52
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	7	0.52
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	1	0.52
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE1	7	0.52
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE2	7	0.52
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	4	0.51
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	4	0.51
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	11	0.51
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	11	0.51
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	19	0.51
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	10	0.51
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	10	0.51
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	18	0.51
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	18	0.51
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	11	0.51
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	10	0.51
(1,717)	1:5:A:PRO:HD3	1:6:A:GLU:H	8	0.51
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	7	0.51
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	7	0.51
(1,646)	1:76:A:VAL:H	1:76:A:VAL:HB	15	0.51
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	6	0.51
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	3	0.51
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	6	0.51
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	3	0.51
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	15	0.51
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	3	0.51
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	3	0.51
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	3	0.51
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	8	0.5
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	8	0.5
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	12	0.5
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	12	0.5
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	6	0.5
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	17	0.5
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	17	0.5
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	17	0.5
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	17	0.5
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	17	0.5
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	17	0.5
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	19	0.5
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	12	0.5
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	12	0.5
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	12	0.5
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	6	0.5
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	8	0.5
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	7	0.5
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	9	0.5
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	19	0.5
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	10	0.49
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	10	0.49
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	9	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	9	0.49
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	18	0.49
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	18	0.49
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	11	0.49
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	11	0.49
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	11	0.49
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	11	0.49
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	15	0.49
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	15	0.49
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	15	0.49
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	15	0.49
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	15	0.49
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	15	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	18	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	18	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	18	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	18	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	18	0.49
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	18	0.49
(1,1699)	1:42:A:SER:HB3	1:43:A:ILE:HA	12	0.49
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	7	0.49
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	9	0.49
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	9	0.49
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	9	0.49
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	9	0.49
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	9	0.49
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	9	0.49
(1,1499)	1:58:A:CYS:HA	1:59:A:ARG:HD3	7	0.49
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	11	0.49
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	12	0.49
(1,783)	1:17:A:THR:H	1:19:A:GLU:HG2	5	0.49
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	2	0.49
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	18	0.49
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	18	0.49
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	16	0.49
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	12	0.49
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	12	0.49
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	12	0.49
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	2	0.49
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	2	0.49
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	6	0.49
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	16	0.48
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	16	0.48
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	14	0.48
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	14	0.48
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	6	0.48
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	0.48
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD1	13	0.48
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD2	13	0.48
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD1	13	0.48
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD2	13	0.48
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD1	13	0.48
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD2	13	0.48
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	2	0.48
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	2	0.48
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	1	0.48
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	18	0.48
(1,646)	1:76:A:VAL:H	1:76:A:VAL:HB	6	0.48
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	2	0.48
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	11	0.48
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	8	0.48
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	17	0.48
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	17	0.48
(1,139)	1:80:A:ILE:H	1:81:A:GLN:H	10	0.48
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	4	0.48
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	16	0.48
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	4	0.47
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	4	0.47
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	4	0.47
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	4	0.47
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	2	0.47
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	2	0.47
(1,2388)	1:76:A:VAL:HG11	1:78:A:LYS:H	15	0.47
(1,2388)	1:76:A:VAL:HG12	1:78:A:LYS:H	15	0.47
(1,2388)	1:76:A:VAL:HG13	1:78:A:LYS:H	15	0.47
(1,2388)	1:76:A:VAL:HG21	1:78:A:LYS:H	15	0.47
(1,2388)	1:76:A:VAL:HG22	1:78:A:LYS:H	15	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2388)	1:76:A:VAL:HG23	1:78:A:LYS:H	15	0.47
(1,2363)	1:73:A:MET:HG2	1:90:A:CYS:HA	1	0.47
(1,2363)	1:73:A:MET:HG3	1:90:A:CYS:HA	1	0.47
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	14	0.47
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	14	0.47
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	14	0.47
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	13	0.47
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	13	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	11	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	11	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	11	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	11	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	11	0.47
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	11	0.47
(1,2000)	1:6:A:GLU:HG2	1:7:A:TRP:HA	5	0.47
(1,2000)	1:6:A:GLU:HG3	1:7:A:TRP:HA	5	0.47
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG11	11	0.47
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG12	11	0.47
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG13	11	0.47
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	4	0.47
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	4	0.47
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	4	0.47
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	4	0.47
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	4	0.47
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	4	0.47
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	14	0.47
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	14	0.47
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	14	0.47
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	14	0.47
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	14	0.47
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	14	0.47
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	1	0.47
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	1	0.47
(1,1112)	1:33:A:ARG:H	1:36:A:TYR:HB3	19	0.47
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	13	0.47
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	9	0.47
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:17:A:THR:H	1:19:A:GLU:HG3	20	0.47
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	2	0.47
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	2	0.47
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	2	0.47
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	18	0.47
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	15	0.47
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	7	0.46
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	7	0.46
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	7	0.46
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	7	0.46
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	19	0.46
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	19	0.46
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	19	0.46
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	19	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	1	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	1	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	1	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	1	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	1	0.46
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	1	0.46
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	1	0.46
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	17	0.46
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	17	0.46
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG2	12	0.46
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG3	12	0.46
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	4	0.46
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	4	0.46
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	7	0.46
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	7	0.46
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	15	0.46
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	15	0.46
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD3	20	0.46
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD3	20	0.46
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD3	20	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD3	20	0.46
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD3	20	0.46
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD2	20	0.46
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD3	20	0.46
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	15	0.46
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	15	0.46
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	15	0.46
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	15	0.46
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	15	0.46
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	15	0.46
(1,1499)	1:58:A:CYS:HA	1:59:A:ARG:HD3	10	0.46
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	12	0.46
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	12	0.46
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	12	0.46
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	8	0.46
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	17	0.46
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	4	0.46
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	15	0.46
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	15	0.46
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	18	0.46
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	18	0.46
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	18	0.46
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	10	0.46
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	18	0.46
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	1	0.46
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	14	0.46
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD2	2	0.45
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD3	2	0.45
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	18	0.45
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	18	0.45
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	18	0.45
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	18	0.45
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	18	0.45
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	18	0.45
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	4	0.45
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	4	0.45
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	4	0.45
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	4	0.45
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	10	0.45
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	14	0.45
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	14	0.45
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG11	13	0.45
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG12	13	0.45
(1,1916)	1:70:A:VAL:HA	1:70:A:VAL:HG13	13	0.45
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	1	0.45
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	12	0.45
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	12	0.45
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	12	0.45
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	12	0.45
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	12	0.45
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	12	0.45
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	15	0.45
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	15	0.45
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	15	0.45
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	15	0.45
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	15	0.45
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	15	0.45
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	5	0.45
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	0.45
(1,923)	1:15:A:GLN:HE21	1:28:A:LEU:HG	20	0.45
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	3	0.45
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	19	0.45
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	11	0.45
(1,790)	1:16:A:LEU:H	1:28:A:LEU:HG	20	0.45
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	5	0.45
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	5	0.45
(1,571)	1:81:A:GLN:H	1:84:A:SER:H	1	0.45
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	11	0.45
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	12	0.45
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	3	0.45
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	12	0.45
(1,2472)	1:92:A:LYS:HA	1:92:A:LYS:HE2	5	0.44
(1,2472)	1:92:A:LYS:HA	1:92:A:LYS:HE3	5	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	20	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	20	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	20	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	20	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	20	0.44
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	20	0.44
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	20	0.44
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	20	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	20	0.44
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	20	0.44
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	20	0.44
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	20	0.44
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	3	0.44
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	3	0.44
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	8	0.44
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	8	0.44
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	1	0.44
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	1	0.44
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	13	0.44
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	13	0.44
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	6	0.44
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	6	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD11	13	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD12	13	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD13	13	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD21	13	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD22	13	0.44
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD23	13	0.44
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	17	0.44
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	13	0.44
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	13	0.44
(1,1499)	1:58:A:CYS:HA	1:59:A:ARG:HD3	15	0.44
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	1	0.44
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	19	0.44
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	19	0.44
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	10	0.44
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	6	0.44
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	13	0.44
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	18	0.44
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	3	0.44
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	3	0.44
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	3	0.44
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	20	0.44
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	13	0.44
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	1	0.44
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE2	9	0.43
(1,2470)	1:92:A:LYS:H	1:92:A:LYS:HE3	9	0.43
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	15	0.43
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	15	0.43
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD2	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2219)	1:57:A:ARG:HA	1:57:A:ARG:HD3	19	0.43
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	11	0.43
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	11	0.43
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	16	0.43
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	16	0.43
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	12	0.43
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	16	0.43
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	1	0.43
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	1	0.43
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	1	0.43
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	1	0.43
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	1	0.43
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	1	0.43
(1,1421)	1:112:A:ILE:HA	1:112:A:ILE:HG21	7	0.43
(1,1421)	1:112:A:ILE:HA	1:112:A:ILE:HG22	7	0.43
(1,1421)	1:112:A:ILE:HA	1:112:A:ILE:HG23	7	0.43
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	10	0.43
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	10	0.43
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	10	0.43
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	3	0.43
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	3	0.43
(1,861)	1:41:A:PHE:HA	1:42:A:SER:H	2	0.43
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	7	0.43
(1,795)	1:18:A:ASP:H	1:19:A:GLU:HG3	17	0.43
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	18	0.43
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	8	0.43
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	8	0.43
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	8	0.43
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	10	0.43
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	1	0.43
(1,133)	1:79:A:GLY:H	1:80:A:ILE:H	1	0.43
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB2	8	0.42
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB3	8	0.42
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	11	0.42
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	11	0.42
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	12	0.42
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	12	0.42
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	13	0.42
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	13	0.42
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	2	0.42
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	2	0.42
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	2	0.42
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	4	0.42
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	4	0.42
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	11	0.42
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	11	0.42
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	17	0.42
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	17	0.42
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	17	0.42
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	17	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	3	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	3	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	3	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	3	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	3	0.42
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	3	0.42
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	15	0.42
(1,1814)	1:73:A:MET:HE1	1:92:A:LYS:H	14	0.42
(1,1814)	1:73:A:MET:HE2	1:92:A:LYS:H	14	0.42
(1,1814)	1:73:A:MET:HE3	1:92:A:LYS:H	14	0.42
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG21	10	0.42
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG22	10	0.42
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG23	10	0.42
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	7	0.42
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	7	0.42
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	7	0.42
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	10	0.42
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	10	0.42
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	10	0.42
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	12	0.42
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	9	0.42
(1,861)	1:41:A:PHE:HA	1:42:A:SER:H	3	0.42
(1,844)	1:28:A:LEU:HD11	1:29:A:ASN:H	11	0.42
(1,844)	1:28:A:LEU:HD12	1:29:A:ASN:H	11	0.42
(1,844)	1:28:A:LEU:HD13	1:29:A:ASN:H	11	0.42
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	17	0.42
(1,760)	1:50:A:VAL:H	1:51:A:TRP:H	1	0.42
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	3	0.42
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	3	0.42
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	3	0.42
(1,692)	1:61:A:LYS:H	1:81:A:GLN:HE21	16	0.42
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	12	0.42
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	12	0.42
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	19	0.42
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	20	0.42
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	1	0.42
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	15	0.42
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	4	0.41
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	4	0.41
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	4	0.41
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	4	0.41
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	18	0.41
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	18	0.41
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	19	0.41
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	19	0.41
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	4	0.41
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	4	0.41
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	3	0.41
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	3	0.41
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	20	0.41
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	20	0.41
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	20	0.41
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	20	0.41
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	17	0.41
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	17	0.41
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG2	3	0.41
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG3	3	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	10	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	10	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	10	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	10	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	10	0.41
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	10	0.41
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	10	0.41
(1,1807)	1:42:A:SER:HA	1:43:A:ILE:HG21	12	0.41
(1,1807)	1:42:A:SER:HA	1:43:A:ILE:HG22	12	0.41
(1,1807)	1:42:A:SER:HA	1:43:A:ILE:HG23	12	0.41
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	15	0.41
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	20	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	20	0.41
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	20	0.41
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	20	0.41
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	20	0.41
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	20	0.41
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	16	0.41
(1,1475)	1:76:A:VAL:HB	1:80:A:ILE:HA	12	0.41
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	6	0.41
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	17	0.41
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	17	0.41
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	17	0.41
(1,847)	1:38:A:GLY:HA2	1:39:A:ARG:H	11	0.41
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	15	0.41
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	4	0.41
(1,261)	1:54:A:ALA:H	1:55:A:LYS:H	5	0.41
(1,157)	1:37:A:SER:H	1:38:A:GLY:H	7	0.41
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	12	0.41
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	19	0.41
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	19	0.41
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	19	0.41
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	20	0.41
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	20	0.41
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	2	0.41
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	13	0.41
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD13	9	0.4
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD13	9	0.4
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD13	9	0.4
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD13	9	0.4
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD13	9	0.4
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD11	9	0.4
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD12	9	0.4
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD13	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	4	0.4
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	4	0.4
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	17	0.4
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	17	0.4
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	17	0.4
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	17	0.4
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	20	0.4
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	20	0.4
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	12	0.4
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	12	0.4
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	5	0.4
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	5	0.4
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	9	0.4
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	9	0.4
(1,2163)	1:47:A:LYS:HG2	1:48:A:ASN:H	1	0.4
(1,2163)	1:47:A:LYS:HG3	1:48:A:ASN:H	1	0.4
(1,2134)	1:41:A:PHE:HB2	1:42:A:SER:H	9	0.4
(1,2134)	1:41:A:PHE:HB3	1:42:A:SER:H	9	0.4
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	7	0.4
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	7	0.4
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	4	0.4
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	4	0.4
(1,2015)	1:8:A:LEU:HD11	1:9:A:PRO:HD3	18	0.4
(1,2015)	1:8:A:LEU:HD12	1:9:A:PRO:HD3	18	0.4
(1,2015)	1:8:A:LEU:HD13	1:9:A:PRO:HD3	18	0.4
(1,2015)	1:8:A:LEU:HD21	1:9:A:PRO:HD3	18	0.4
(1,2015)	1:8:A:LEU:HD22	1:9:A:PRO:HD3	18	0.4
(1,2015)	1:8:A:LEU:HD23	1:9:A:PRO:HD3	18	0.4
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	10	0.4
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	19	0.4
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	19	0.4
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	19	0.4
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	13	0.4
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	3	0.4
(1,771)	1:51:A:TRP:H	1:51:A:TRP:HB2	19	0.4
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	1	0.4
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	1	0.4
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	17	0.4
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	20	0.4
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	4	0.4
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	15	0.4
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	20	0.4
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	2	0.4
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	19	0.4
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	8	0.4
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	8	0.4
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	12	0.39
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	12	0.39
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	12	0.39
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	12	0.39
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	12	0.39
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	12	0.39
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	5	0.39
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	5	0.39
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	5	0.39
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	5	0.39
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	20	0.39
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	20	0.39
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	11	0.39
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	11	0.39
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	9	0.39
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	9	0.39
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	10	0.39
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	10	0.39
(1,2111)	1:36:A:TYR:HD1	1:37:A:SER:HB2	7	0.39
(1,2111)	1:36:A:TYR:HD1	1:37:A:SER:HB3	7	0.39
(1,2111)	1:36:A:TYR:HD2	1:37:A:SER:HB2	7	0.39
(1,2111)	1:36:A:TYR:HD2	1:37:A:SER:HB3	7	0.39
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	19	0.39
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	19	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD11	8	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD12	8	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD13	8	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD21	8	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD22	8	0.39
(1,2049)	1:15:A:GLN:HE22	1:16:A:LEU:HD23	8	0.39
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	6	0.39
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	6	0.39
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	12	0.39
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	12	0.39
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	12	0.39
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	12	0.39
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	12	0.39
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	19	0.39
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	19	0.39
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB2	13	0.39
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB3	13	0.39
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	19	0.39
(1,952)	1:107:A:SER:H	1:110:A:THR:H	14	0.39
(1,892)	1:3:A:ASN:HD21	1:4:A:ALA:H	17	0.39
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	18	0.39
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	4	0.39
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	4	0.39
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	5	0.39
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	4	0.39
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	4	0.39
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	4	0.39
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	5	0.39
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	5	0.39
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	5	0.39
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	5	0.39
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	8	0.39
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	8	0.39
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	7	0.39
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	9	0.39
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	16	0.39
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	7	0.39
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	14	0.39
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	7	0.39
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	7	0.39
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	17	0.38
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	17	0.38
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	20	0.38
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	20	0.38
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	6	0.38
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	6	0.38
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	1	0.38
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	1	0.38
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	12	0.38
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	12	0.38
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	13	0.38
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	13	0.38
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	18	0.38
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	18	0.38
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	18	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	12	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	14	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	14	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	14	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	14	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	14	0.38
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	14	0.38
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG2	18	0.38
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG3	18	0.38
(1,1882)	1:28:A:LEU:HB3	1:29:A:ASN:HB3	20	0.38
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	8	0.38
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	4	0.38
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	4	0.38
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	4	0.38
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	9	0.38
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	18	0.38
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	18	0.38
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	18	0.38
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	1	0.38
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	1	0.38
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	4	0.38
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	11	0.38
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	11	0.38
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	11	0.38
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	11	0.38
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	11	0.38
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	11	0.38
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	15	0.38
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	20	0.38
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	20	0.38
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	20	0.38
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	5	0.38
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	5	0.38
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	5	0.38
(1,960)	1:51:A:TRP:H	1:51:A:TRP:HD1	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	14	0.38
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	18	0.38
(1,884)	1:2:A:CYS:HA	1:51:A:TRP:HE1	15	0.38
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	3	0.38
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	19	0.38
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	9	0.38
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	9	0.38
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	9	0.38
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	5	0.38
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	7	0.38
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	17	0.38
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	4	0.38
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	12	0.38
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	15	0.38
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	15	0.38
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	5	0.38
(1,161)	1:14:A:THR:H	1:29:A:ASN:H	19	0.38
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	2	0.38
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	4	0.38
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	7	0.37
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	7	0.37
(1,2481)	1:92:A:LYS:HE2	1:93:A:GLY:H	18	0.37
(1,2481)	1:92:A:LYS:HE3	1:93:A:GLY:H	18	0.37
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	19	0.37
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	19	0.37
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	16	0.37
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	16	0.37
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	19	0.37
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	19	0.37
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	11	0.37
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	11	0.37
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	4	0.37
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	4	0.37
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	19	0.37
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	19	0.37
(1,2165)	1:47:A:LYS:HG2	1:49:A:SER:H	1	0.37
(1,2165)	1:47:A:LYS:HG3	1:49:A:SER:H	1	0.37
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	14	0.37
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	14	0.37
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	16	0.37
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	16	0.37
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	16	0.37
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	16	0.37
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	16	0.37
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	12	0.37
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	12	0.37
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	12	0.37
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	7	0.37
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	8	0.37
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	8	0.37
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	8	0.37
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	17	0.37
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	17	0.37
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	10	0.37
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	11	0.37
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	9	0.37
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	2	0.37
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	20	0.37
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	2	0.37
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	5	0.37
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	1	0.37
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	4	0.37
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	3	0.37
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	17	0.37
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	9	0.37
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	5	0.37
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	11	0.37
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	11	0.37
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	11	0.37
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	2	0.37
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	2	0.37
(1,148)	1:74:A:VAL:HG11	1:89:A:SER:H	14	0.37
(1,148)	1:74:A:VAL:HG12	1:89:A:SER:H	14	0.37
(1,148)	1:74:A:VAL:HG13	1:89:A:SER:H	14	0.37
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	10	0.37
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	5	0.37
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	5	0.37
(1,81)	1:60:A:ARG:H	1:60:A:ARG:HD3	19	0.37
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	8	0.37
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	16	0.36
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	16	0.36
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	16	0.36
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	16	0.36
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	16	0.36
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	16	0.36
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	18	0.36
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	18	0.36
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	2	0.36
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	2	0.36
(1,2399)	1:77:A:ILE:HG21	1:78:A:LYS:HE2	20	0.36
(1,2399)	1:77:A:ILE:HG21	1:78:A:LYS:HE3	20	0.36
(1,2399)	1:77:A:ILE:HG22	1:78:A:LYS:HE2	20	0.36
(1,2399)	1:77:A:ILE:HG22	1:78:A:LYS:HE3	20	0.36
(1,2399)	1:77:A:ILE:HG23	1:78:A:LYS:HE2	20	0.36
(1,2399)	1:77:A:ILE:HG23	1:78:A:LYS:HE3	20	0.36
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	17	0.36
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	17	0.36
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	3	0.36
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	3	0.36
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	5	0.36
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	5	0.36
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG2	7	0.36
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG3	7	0.36
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG2	1	0.36
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG3	1	0.36
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG2	1	0.36
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG3	1	0.36
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	17	0.36
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	17	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	8	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	8	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	8	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	8	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	8	0.36
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	8	0.36
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	15	0.36
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	15	0.36
(1,1993)	1:5:A:PRO:HB3	1:6:A:GLU:HG2	18	0.36
(1,1993)	1:5:A:PRO:HB3	1:6:A:GLU:HG3	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG2	6	0.36
(1,1992)	1:5:A:PRO:HB2	1:6:A:GLU:HG3	6	0.36
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	15	0.36
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	15	0.36
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	15	0.36
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	15	0.36
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	15	0.36
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	15	0.36
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE1	11	0.36
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE2	11	0.36
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE3	11	0.36
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	11	0.36
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	14	0.36
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	18	0.36
(1,1708)	1:10:A:PHE:HE1	1:55:A:LYS:HA	7	0.36
(1,1708)	1:10:A:PHE:HE2	1:55:A:LYS:HA	7	0.36
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	8	0.36
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	14	0.36
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	16	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	4	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	4	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	4	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	4	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	4	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	4	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	16	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	16	0.36
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	16	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	16	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	16	0.36
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	16	0.36
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	6	0.36
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	6	0.36
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	20	0.36
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	16	0.36
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	6	0.36
(1,1096)	1:17:A:THR:HG21	1:19:A:GLU:HG3	17	0.36
(1,1096)	1:17:A:THR:HG22	1:19:A:GLU:HG3	17	0.36
(1,1096)	1:17:A:THR:HG23	1:19:A:GLU:HG3	17	0.36
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	1	0.36
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	1	0.36
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	2	0.36
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	2	0.36
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	2	0.36
(1,952)	1:107:A:SER:H	1:110:A:THR:H	18	0.36
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	14	0.36
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	14	0.36
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	13	0.36
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	11	0.36
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	20	0.36
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	13	0.36
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	15	0.36
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	2	0.36
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	2	0.36
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	19	0.36
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	7	0.36
(1,657)	1:73:A:MET:H	1:88:A:TYR:HD1	17	0.36
(1,657)	1:73:A:MET:H	1:88:A:TYR:HD2	17	0.36
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	11	0.36
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	4	0.36
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	17	0.36
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	20	0.36
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	9	0.36
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	10	0.36
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	12	0.36
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	4	0.36
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	19	0.36
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB2	2	0.35
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB3	2	0.35
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	5	0.35
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	5	0.35
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	7	0.35
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	7	0.35
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	14	0.35
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	14	0.35
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	5	0.35
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	5	0.35
(1,2134)	1:41:A:PHE:HB2	1:42:A:SER:H	1	0.35
(1,2134)	1:41:A:PHE:HB3	1:42:A:SER:H	1	0.35
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG2	14	0.35
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG3	14	0.35
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG2	14	0.35
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG3	14	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	8	0.35
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	8	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	11	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	11	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	11	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	11	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	11	0.35
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	11	0.35
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	11	0.35
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	20	0.35
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	20	0.35
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	20	0.35
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	20	0.35
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	20	0.35
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	20	0.35
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	20	0.35
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	13	0.35
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	13	0.35
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	13	0.35
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	19	0.35
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	19	0.35
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	19	0.35
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	5	0.35
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	7	0.35
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	2	0.35
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	6	0.35
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	6	0.35
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	6	0.35
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	7	0.35
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	10	0.35
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	13	0.35
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	15	0.35
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	15	0.35
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	9	0.35
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	11	0.35
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	11	0.35
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	11	0.35
(1,1129)	1:122:A:ARG:H	1:122:A:ARG:HB3	9	0.35
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	19	0.35
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	19	0.35
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	19	0.35
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	8	0.35
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	16	0.35
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	7	0.35
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	11	0.35
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	4	0.35
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	4	0.35
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	10	0.35
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	10	0.35
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	10	0.35
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	3	0.35
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	20	0.35
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	18	0.35
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	7	0.35
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	17	0.35
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	1	0.35
(1,237)	1:8:A:LEU:HB2	1:11:A:ALA:H	18	0.35
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	6	0.35
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	6	0.35
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	6	0.35
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	8	0.35
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	8	0.35
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	8	0.35
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	1	0.35
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	16	0.35
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	20	0.35
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	20	0.35
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	20	0.35
(1,2491)	1:95:A:ARG:HG2	1:121:A:ASP:HA	10	0.34
(1,2491)	1:95:A:ARG:HG3	1:121:A:ASP:HA	10	0.34
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	8	0.34
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	8	0.34
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	2	0.34
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	8	0.34
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	8	0.34
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	19	0.34
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	19	0.34
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	16	0.34
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	16	0.34
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	11	0.34
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	11	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	6	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	6	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	16	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	16	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	20	0.34
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	20	0.34
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	6	0.34
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	6	0.34
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	7	0.34
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	7	0.34
(1,2166)	1:47:A:LYS:HG2	1:50:A:VAL:H	8	0.34
(1,2166)	1:47:A:LYS:HG3	1:50:A:VAL:H	8	0.34
(1,2165)	1:47:A:LYS:HG2	1:49:A:SER:H	8	0.34
(1,2165)	1:47:A:LYS:HG3	1:49:A:SER:H	8	0.34
(1,2116)	1:37:A:SER:HB2	1:38:A:GLY:H	14	0.34
(1,2116)	1:37:A:SER:HB3	1:38:A:GLY:H	14	0.34
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	6	0.34
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	6	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	9	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	9	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	9	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	9	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	9	0.34
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	9	0.34
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	19	0.34
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	19	0.34
(1,1885)	1:8:A:LEU:HD11	1:10:A:PHE:HE1	17	0.34
(1,1885)	1:8:A:LEU:HD11	1:10:A:PHE:HE2	17	0.34
(1,1885)	1:8:A:LEU:HD12	1:10:A:PHE:HE1	17	0.34
(1,1885)	1:8:A:LEU:HD12	1:10:A:PHE:HE2	17	0.34
(1,1885)	1:8:A:LEU:HD13	1:10:A:PHE:HE1	17	0.34
(1,1885)	1:8:A:LEU:HD13	1:10:A:PHE:HE2	17	0.34
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	2	0.34
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	2	0.34
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	15	0.34
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	15	0.34
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	15	0.34
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	1	0.34
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	16	0.34
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	16	0.34
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	16	0.34
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	15	0.34
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	15	0.34
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	15	0.34
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	11	0.34
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG2	6	0.34
(1,1626)	1:14:A:THR:HG21	1:15:A:GLN:HG3	6	0.34
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG2	6	0.34
(1,1626)	1:14:A:THR:HG22	1:15:A:GLN:HG3	6	0.34
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG2	6	0.34
(1,1626)	1:14:A:THR:HG23	1:15:A:GLN:HG3	6	0.34
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	2	0.34
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	2	0.34
(1,1553)	1:96:A:LEU:HD21	1:119:A:ILE:H	7	0.34
(1,1553)	1:96:A:LEU:HD22	1:119:A:ILE:H	7	0.34
(1,1553)	1:96:A:LEU:HD23	1:119:A:ILE:H	7	0.34
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	1	0.34
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	1	0.34
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	1	0.34
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	3	0.34
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	3	0.34
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	3	0.34
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	16	0.34
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	7	0.34
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	18	0.34
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	18	0.34
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	18	0.34
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	7	0.34
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	3	0.34
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	3	0.34
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	3	0.34
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	9	0.34
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	20	0.34
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	13	0.34
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	13	0.34
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	8	0.34
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	18	0.34
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	12	0.34
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	15	0.34
(1,372)	1:13:A:PRO:HB2	1:30:A:TYR:H	18	0.34
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	16	0.34
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	19	0.34
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	19	0.34
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	19	0.34
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD13	11	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD13	11	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD13	11	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD13	11	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD13	11	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD11	11	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD12	11	0.33
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD13	11	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	1	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	1	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	1	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	1	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	1	0.33
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	1	0.33
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	14	0.33
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	14	0.33
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	14	0.33
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	14	0.33
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	12	0.33
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	12	0.33
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	6	0.33
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	7	0.33
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	7	0.33
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	9	0.33
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	9	0.33
(1,2267)	1:61:A:LYS:HG2	1:62:A:SER:HA	10	0.33
(1,2267)	1:61:A:LYS:HG3	1:62:A:SER:HA	10	0.33
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	17	0.33
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	17	0.33
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	2	0.33
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	2	0.33
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	15	0.33
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	15	0.33
(1,2161)	1:47:A:LYS:HB2	1:52:A:THR:HA	10	0.33
(1,2161)	1:47:A:LYS:HB3	1:52:A:THR:HA	10	0.33
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	9	0.33
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	9	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	7	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	15	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	17	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	17	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	17	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	17	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	17	0.33
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	17	0.33
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	1	0.33
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	15	0.33
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	15	0.33
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	15	0.33
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	15	0.33
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	15	0.33
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	15	0.33
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	15	0.33
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	15	0.33
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	7	0.33
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE1	19	0.33
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE2	19	0.33
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE3	19	0.33
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	16	0.33
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	11	0.33
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	11	0.33
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	11	0.33
(1,1322)	1:96:A:LEU:HD11	1:119:A:ILE:HD11	12	0.33
(1,1322)	1:96:A:LEU:HD11	1:119:A:ILE:HD12	12	0.33
(1,1322)	1:96:A:LEU:HD11	1:119:A:ILE:HD13	12	0.33
(1,1322)	1:96:A:LEU:HD12	1:119:A:ILE:HD11	12	0.33
(1,1322)	1:96:A:LEU:HD12	1:119:A:ILE:HD12	12	0.33
(1,1322)	1:96:A:LEU:HD12	1:119:A:ILE:HD13	12	0.33
(1,1322)	1:96:A:LEU:HD13	1:119:A:ILE:HD11	12	0.33
(1,1322)	1:96:A:LEU:HD13	1:119:A:ILE:HD12	12	0.33
(1,1322)	1:96:A:LEU:HD13	1:119:A:ILE:HD13	12	0.33
(1,1295)	1:92:A:LYS:H	1:92:A:LYS:HB2	20	0.33
(1,1232)	1:22:A:PHE:HD1	1:51:A:TRP:HZ2	2	0.33
(1,1232)	1:22:A:PHE:HD2	1:51:A:TRP:HZ2	2	0.33
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	18	0.33
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD11	10	0.33
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD12	10	0.33
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD13	10	0.33
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD11	10	0.33
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD12	10	0.33
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD13	10	0.33
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD11	10	0.33
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD12	10	0.33
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD13	10	0.33
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	9	0.33
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	9	0.33
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	9	0.33
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG21	16	0.33
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG22	16	0.33
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG23	16	0.33
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	6	0.33
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	19	0.33
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	6	0.33
(1,760)	1:50:A:VAL:H	1:51:A:TRP:H	14	0.33
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	16	0.33
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	18	0.33
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	16	0.33
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	16	0.33
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	16	0.33
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	2	0.33
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	2	0.33
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	15	0.33
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	14	0.33
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	13	0.33
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	9	0.33
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	14	0.33
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	10	0.33
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	7	0.33
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	20	0.33
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	15	0.33
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	3	0.33
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	6	0.33
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	18	0.33
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	13	0.33
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	13	0.33
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	13	0.33
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	9	0.33
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	13	0.33
(1,48)	1:12:A:ARG:H	1:32:A:CYS:H	1	0.33
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	10	0.33
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	10	0.33
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	10	0.33
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	10	0.32
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	10	0.32
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	10	0.32
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	10	0.32
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	4	0.32
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	4	0.32
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	4	0.32
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	4	0.32
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	8	0.32
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	8	0.32
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	8	0.32
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	8	0.32
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	8	0.32
(1,2478)	1:92:A:LYS:HD2	1:93:A:GLY:H	10	0.32
(1,2478)	1:92:A:LYS:HD3	1:93:A:GLY:H	10	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	8	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	8	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	8	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	8	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	8	0.32
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	8	0.32
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	8	0.32
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	12	0.32
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	12	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	3	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	3	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	6	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	6	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	13	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	13	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	17	0.32
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	17	0.32
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	10	0.32
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	10	0.32
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	13	0.32
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	13	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG11	19	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG12	19	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG13	19	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG21	19	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG22	19	0.32
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG23	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG11	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG12	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG13	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG21	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG22	19	0.32
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG23	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	18	0.32
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	18	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	3	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	3	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	3	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	3	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	11	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	11	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	11	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	11	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	17	0.32
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	17	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	17	0.32
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	17	0.32
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	7	0.32
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	7	0.32
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	7	0.32
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	7	0.32
(1,2252)	1:60:A:ARG:HD2	1:82:A:PHE:HA	18	0.32
(1,2252)	1:60:A:ARG:HD3	1:82:A:PHE:HA	18	0.32
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	19	0.32
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	19	0.32
(1,2165)	1:47:A:LYS:HG2	1:49:A:SER:H	17	0.32
(1,2165)	1:47:A:LYS:HG3	1:49:A:SER:H	17	0.32
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	18	0.32
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	18	0.32
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	18	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	5	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	8	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	8	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	8	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	8	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	8	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	20	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	20	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	20	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	20	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	20	0.32
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	20	0.32
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	8	0.32
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	8	0.32
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	9	0.32
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	4	0.32
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	4	0.32
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	10	0.32
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	10	0.32
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	10	0.32
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	3	0.32
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	4	0.32
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	14	0.32
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	14	0.32
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	14	0.32
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	9	0.32
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	9	0.32
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	4	0.32
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	4	0.32
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	4	0.32
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	1	0.32
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	1	0.32
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	1	0.32
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	3	0.32
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	4	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	5	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	5	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	5	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	8	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	8	0.32
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	8	0.32
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	2	0.32
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	2	0.32
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	3	0.32
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	3	0.32
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:4:A:ALA:HB1	1:51:A:TRP:HZ2	10	0.32
(1,1240)	1:4:A:ALA:HB2	1:51:A:TRP:HZ2	10	0.32
(1,1240)	1:4:A:ALA:HB3	1:51:A:TRP:HZ2	10	0.32
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	11	0.32
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	11	0.32
(1,1148)	1:36:A:TYR:HA	1:60:A:ARG:HA	1	0.32
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	12	0.32
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	12	0.32
(1,960)	1:51:A:TRP:H	1:51:A:TRP:HD1	8	0.32
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	16	0.32
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	14	0.32
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	14	0.32
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	14	0.32
(1,856)	1:35:A:GLY:H	1:36:A:TYR:HB2	7	0.32
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	12	0.32
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	13	0.32
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	2	0.32
(1,771)	1:51:A:TRP:H	1:51:A:TRP:HB2	8	0.32
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	15	0.32
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	15	0.32
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	15	0.32
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	5	0.32
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	6	0.32
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	1	0.32
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	1	0.32
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	1	0.32
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	11	0.32
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	1	0.32
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	12	0.32
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	20	0.32
(1,485)	1:88:A:TYR:HB3	1:100:A:SER:H	13	0.32
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	2	0.32
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	18	0.32
(1,345)	1:40:A:PRO:HA	1:41:A:PHE:H	17	0.32
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	20	0.32
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	9	0.32
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	9	0.32
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	9	0.32
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	1	0.32
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	11	0.32
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	11	0.32
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	7	0.32
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	15	0.32
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	3	0.32
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	3	0.32
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	3	0.32
(1,2573)	1:116:A:GLU:HB2	1:117:A:THR:H	3	0.31
(1,2573)	1:116:A:GLU:HB3	1:117:A:THR:H	3	0.31
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	8	0.31
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	8	0.31
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	5	0.31
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	5	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	12	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	12	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	12	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	12	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	12	0.31
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	12	0.31
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	12	0.31
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD11	13	0.31
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD12	13	0.31
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD13	13	0.31
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD11	13	0.31
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD12	13	0.31
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD13	13	0.31
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	15	0.31
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	15	0.31
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	20	0.31
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	20	0.31
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	14	0.31
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	14	0.31
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	14	0.31
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	14	0.31
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	1	0.31
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	1	0.31
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	3	0.31
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	3	0.31
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	16	0.31
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	18	0.31
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	18	0.31
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	16	0.31
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	16	0.31
(1,2138)	1:43:A:ILE:HG21	1:57:A:ARG:HD2	20	0.31
(1,2138)	1:43:A:ILE:HG21	1:57:A:ARG:HD3	20	0.31
(1,2138)	1:43:A:ILE:HG22	1:57:A:ARG:HD2	20	0.31
(1,2138)	1:43:A:ILE:HG22	1:57:A:ARG:HD3	20	0.31
(1,2138)	1:43:A:ILE:HG23	1:57:A:ARG:HD2	20	0.31
(1,2138)	1:43:A:ILE:HG23	1:57:A:ARG:HD3	20	0.31
(1,2134)	1:41:A:PHE:HB2	1:42:A:SER:H	8	0.31
(1,2134)	1:41:A:PHE:HB3	1:42:A:SER:H	8	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	3	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	19	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	19	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	19	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	19	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	19	0.31
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	19	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	4	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	4	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	4	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	4	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	4	0.31
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	4	0.31
(1,2001)	1:6:A:GLU:HG2	1:8:A:LEU:H	5	0.31
(1,2001)	1:6:A:GLU:HG3	1:8:A:LEU:H	5	0.31
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG2	5	0.31
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG3	5	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	1	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	1	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	1	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	1	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	1	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	1	0.31
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	1	0.31
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	1	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	11	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	11	0.31
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	11	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	11	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	11	0.31
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	11	0.31
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	11	0.31
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	11	0.31
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	11	0.31
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	10	0.31
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	10	0.31
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	10	0.31
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	6	0.31
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	6	0.31
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	6	0.31
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	18	0.31
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	6	0.31
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	6	0.31
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	6	0.31
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	10	0.31
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	5	0.31
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	5	0.31
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	5	0.31
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	17	0.31
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	17	0.31
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	17	0.31
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	17	0.31
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	17	0.31
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	17	0.31
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	7	0.31
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	7	0.31
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	7	0.31
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	3	0.31
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	3	0.31
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	3	0.31
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	19	0.31
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	19	0.31
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	19	0.31
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	18	0.31
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	18	0.31
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	2	0.31
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	14	0.31
(1,1325)	1:60:A:ARG:H	1:60:A:ARG:HD2	1	0.31
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	4	0.31
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	1	0.31
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	1	0.31
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	1	0.31
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	2	0.31
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	2	0.31
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	2	0.31
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	11	0.31
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	11	0.31
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	11	0.31
(1,919)	1:13:A:PRO:HB2	1:15:A:GLN:HE22	8	0.31
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	5	0.31
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	2	0.31
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	16	0.31
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	9	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	7	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	7	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	7	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	12	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	12	0.31
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	12	0.31
(1,674)	1:64:A:ARG:HG2	1:65:A:ASN:H	5	0.31
(1,674)	1:64:A:ARG:HG3	1:65:A:ASN:H	5	0.31
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	10	0.31
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	3	0.31
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	3	0.31
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	3	0.31
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	3	0.31
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	6	0.31
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	13	0.31
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	8	0.31
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	17	0.31
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	3	0.31
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	4	0.31
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	5	0.31
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	4	0.31
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	15	0.31
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	1	0.31
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	1	0.31
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	1	0.31
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	7	0.31
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	7	0.31
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	7	0.31
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB2	13	0.3
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB3	13	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	6	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	6	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	6	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	6	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	17	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	17	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	17	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	17	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	19	0.3
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	19	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	19	0.3
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	19	0.3
(1,2428)	1:84:A:SER:HB2	1:104:A:CYS:H	15	0.3
(1,2428)	1:84:A:SER:HB3	1:104:A:CYS:H	15	0.3
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	18	0.3
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	18	0.3
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	5	0.3
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	5	0.3
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	14	0.3
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	14	0.3
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG21	18	0.3
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG22	18	0.3
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG23	18	0.3
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG21	18	0.3
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG22	18	0.3
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG23	18	0.3
(1,2305)	1:64:A:ARG:HD2	1:113:A:TRP:HE1	1	0.3
(1,2305)	1:64:A:ARG:HD3	1:113:A:TRP:HE1	1	0.3
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	1	0.3
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	1	0.3
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG11	11	0.3
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG12	11	0.3
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG13	11	0.3
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG11	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG12	11	0.3
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG13	11	0.3
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	15	0.3
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	15	0.3
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	15	0.3
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	15	0.3
(1,2166)	1:47:A:LYS:HG2	1:50:A:VAL:H	17	0.3
(1,2166)	1:47:A:LYS:HG3	1:50:A:VAL:H	17	0.3
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	1	0.3
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	1	0.3
(1,2116)	1:37:A:SER:HB2	1:38:A:GLY:H	17	0.3
(1,2116)	1:37:A:SER:HB3	1:38:A:GLY:H	17	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	7	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	7	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	7	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	7	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	7	0.3
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	7	0.3
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	7	0.3
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB2	2	0.3
(1,2083)	1:26:A:THR:H	1:45:A:CYS:HB3	2	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	5	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	8	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	8	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	8	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	8	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	8	0.3
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	8	0.3
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	18	0.3
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	18	0.3
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	18	0.3
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD21	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD22	18	0.3
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD23	18	0.3
(1,2031)	1:8:A:LEU:HD11	1:57:A:ARG:HA	20	0.3
(1,2031)	1:8:A:LEU:HD12	1:57:A:ARG:HA	20	0.3
(1,2031)	1:8:A:LEU:HD13	1:57:A:ARG:HA	20	0.3
(1,2031)	1:8:A:LEU:HD21	1:57:A:ARG:HA	20	0.3
(1,2031)	1:8:A:LEU:HD22	1:57:A:ARG:HA	20	0.3
(1,2031)	1:8:A:LEU:HD23	1:57:A:ARG:HA	20	0.3
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	13	0.3
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	13	0.3
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	14	0.3
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	14	0.3
(1,1952)	1:36:A:TYR:HE1	1:61:A:LYS:H	4	0.3
(1,1952)	1:36:A:TYR:HE2	1:61:A:LYS:H	4	0.3
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	16	0.3
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	10	0.3
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	10	0.3
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	10	0.3
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	13	0.3
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	13	0.3
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	13	0.3
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	17	0.3
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	19	0.3
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	19	0.3
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	9	0.3
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	9	0.3
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	9	0.3
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	10	0.3
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	10	0.3
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	10	0.3
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	12	0.3
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	12	0.3
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	12	0.3
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	9	0.3
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	5	0.3
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	11	0.3
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	11	0.3
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	2	0.3
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	6	0.3
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	6	0.3
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	6	0.3
(1,1217)	1:105:A:ILE:HD11	1:114:A:ASP:HB3	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1217)	1:105:A:ILE:HD12	1:114:A:ASP:HB3	19	0.3
(1,1217)	1:105:A:ILE:HD13	1:114:A:ASP:HB3	19	0.3
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	6	0.3
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	16	0.3
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	16	0.3
(1,1044)	1:2:A:CYS:HB2	1:51:A:TRP:HD1	10	0.3
(1,952)	1:107:A:SER:H	1:110:A:THR:H	9	0.3
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	17	0.3
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	16	0.3
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	16	0.3
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD1	8	0.3
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD2	8	0.3
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	2	0.3
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	9	0.3
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	19	0.3
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	5	0.3
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	12	0.3
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	5	0.3
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	13	0.3
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	3	0.3
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	5	0.3
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	4	0.3
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	4	0.3
(1,771)	1:51:A:TRP:H	1:51:A:TRP:HB2	10	0.3
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	1	0.3
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	4	0.3
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	4	0.3
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	4	0.3
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	12	0.3
(1,649)	1:74:A:VAL:H	1:89:A:SER:H	14	0.3
(1,637)	1:26:A:THR:HB	1:45:A:CYS:H	19	0.3
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	3	0.3
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	8	0.3
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	16	0.3
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	9	0.3
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	4	0.3
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	10	0.3
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	13	0.3
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	6	0.3
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	11	0.3
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	13	0.3
(1,180)	1:38:A:GLY:HA3	1:58:A:CYS:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	1	0.3
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	1	0.3
(1,157)	1:37:A:SER:H	1:38:A:GLY:H	3	0.3
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	3	0.3
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	17	0.3
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	17	0.3
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	5	0.3
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	3	0.3
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	3	0.3
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	3	0.3
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	11	0.29
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	11	0.29
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	20	0.29
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	20	0.29
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	20	0.29
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	20	0.29
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	20	0.29
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	20	0.29
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	20	0.29
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	16	0.29
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	16	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	7	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	7	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	7	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	7	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	7	0.29
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	7	0.29
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	7	0.29
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB2	17	0.29
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB3	17	0.29
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	8	0.29
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG2	1	0.29
(1,2355)	1:72:A:GLY:H	1:73:A:MET:HG3	1	0.29
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	16	0.29
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	16	0.29
(1,2283)	1:62:A:SER:HB2	1:64:A:ARG:HB3	11	0.29
(1,2283)	1:62:A:SER:HB3	1:64:A:ARG:HB3	11	0.29
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	5	0.29
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	5	0.29
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	5	0.29
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	5	0.29
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	3	0.29
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	3	0.29
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	9	0.29
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	9	0.29
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	2	0.29
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	2	0.29
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	10	0.29
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	10	0.29
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	10	0.29
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	10	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	13	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	13	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	13	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	13	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	13	0.29
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	13	0.29
(1,1985)	1:3:A:ASN:HA	1:21:A:GLU:HG2	3	0.29
(1,1985)	1:3:A:ASN:HA	1:21:A:GLU:HG3	3	0.29
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	19	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	3	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	3	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	3	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	4	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	4	0.29
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	4	0.29
(1,1750)	1:8:A:LEU:HG	1:10:A:PHE:HB3	18	0.29
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	5	0.29
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	8	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	8	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	8	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	8	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	8	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	8	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	17	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	17	0.29
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	17	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	17	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	17	0.29
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	17	0.29
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	10	0.29
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD11	10	0.29
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD12	10	0.29
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD13	10	0.29
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	19	0.29
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	19	0.29
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	19	0.29
(1,1295)	1:92:A:LYS:H	1:92:A:LYS:HB2	5	0.29
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD1	14	0.29
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD2	14	0.29
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	4	0.29
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	4	0.29
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	2	0.29
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	2	0.29
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	2	0.29
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	7	0.29
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	7	0.29
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	7	0.29
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	13	0.29
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	13	0.29
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	13	0.29
(1,940)	1:63:A:CYS:H	1:63:A:CYS:HB2	17	0.29
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	20	0.29
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	20	0.29
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	20	0.29
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB1	10	0.29
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB2	10	0.29
(1,897)	1:3:A:ASN:HD22	1:4:A:ALA:HB3	10	0.29
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	8	0.29
(1,883)	1:2:A:CYS:HB3	1:51:A:TRP:HE1	2	0.29
(1,862)	1:13:A:PRO:HA	1:31:A:GLU:H	13	0.29
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	16	0.29
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	18	0.29
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	1	0.29
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	5	0.29
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	5	0.29
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	12	0.29
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	6	0.29
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	11	0.29
(1,533)	1:89:A:SER:HA	1:91:A:THR:H	14	0.29
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	1	0.29
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	4	0.29
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	17	0.29
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	19	0.29
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	14	0.29
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	2	0.29
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	18	0.29
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	14	0.29
(1,264)	1:55:A:LYS:H	1:57:A:ARG:HD2	19	0.29
(1,261)	1:54:A:ALA:H	1:55:A:LYS:H	12	0.29
(1,230)	1:112:A:ILE:HB	1:113:A:TRP:H	7	0.29
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	15	0.29
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	13	0.29
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	3	0.29
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	9	0.29
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB2	2	0.28
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB3	2	0.28
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	17	0.28
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	17	0.28
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	17	0.28
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	17	0.28
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	17	0.28
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	17	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	16	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	16	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	16	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	16	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	16	0.28
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	16	0.28
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	5	0.28
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	5	0.28
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	6	0.28
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	6	0.28
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	20	0.28
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	20	0.28
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	20	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	5	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	5	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	5	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	5	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	5	0.28
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	5	0.28
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	5	0.28
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB2	11	0.28
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB3	11	0.28
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	16	0.28
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	16	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	11	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	11	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	14	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	14	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	16	0.28
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	16	0.28
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	17	0.28
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	17	0.28
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	17	0.28
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	17	0.28
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB2	20	0.28
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB3	20	0.28
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	10	0.28
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	10	0.28
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	14	0.28
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	14	0.28
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	14	0.28
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	14	0.28
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	14	0.28
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	14	0.28
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	11	0.28
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	11	0.28
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	13	0.28
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	8	0.28
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	8	0.28
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	8	0.28
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	8	0.28
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	8	0.28
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	8	0.28
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	8	0.28
(1,2055)	1:16:A:LEU:HD11	1:17:A:THR:HA	7	0.28
(1,2055)	1:16:A:LEU:HD12	1:17:A:THR:HA	7	0.28
(1,2055)	1:16:A:LEU:HD13	1:17:A:THR:HA	7	0.28
(1,2055)	1:16:A:LEU:HD21	1:17:A:THR:HA	7	0.28
(1,2055)	1:16:A:LEU:HD22	1:17:A:THR:HA	7	0.28
(1,2055)	1:16:A:LEU:HD23	1:17:A:THR:HA	7	0.28
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG3	2	0.28
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG3	2	0.28
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG3	2	0.28
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG3	2	0.28
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG3	2	0.28
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG2	2	0.28
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG3	2	0.28
(1,2027)	1:8:A:LEU:HD11	1:54:A:ALA:HA	12	0.28
(1,2027)	1:8:A:LEU:HD12	1:54:A:ALA:HA	12	0.28
(1,2027)	1:8:A:LEU:HD13	1:54:A:ALA:HA	12	0.28
(1,2027)	1:8:A:LEU:HD21	1:54:A:ALA:HA	12	0.28
(1,2027)	1:8:A:LEU:HD22	1:54:A:ALA:HA	12	0.28
(1,2027)	1:8:A:LEU:HD23	1:54:A:ALA:HA	12	0.28
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG2	6	0.28
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG3	6	0.28
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	12	0.28
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	12	0.28
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	12	0.28
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	12	0.28
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	12	0.28
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	12	0.28
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	12	0.28
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	12	0.28
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	18	0.28
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	18	0.28
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	18	0.28
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	19	0.28
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	1	0.28
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	1	0.28
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	1	0.28
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	1	0.28
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	3	0.28
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	10	0.28
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	14	0.28
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	14	0.28
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	14	0.28
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	14	0.28
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	14	0.28
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	14	0.28
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	4	0.28
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	12	0.28
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	5	0.28
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	17	0.28
(1,1393)	1:94:A:TYR:HD1	1:122:A:ARG:HA	20	0.28
(1,1393)	1:94:A:TYR:HD2	1:122:A:ARG:HA	20	0.28
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	16	0.28
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	16	0.28
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	16	0.28
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	1	0.28
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	1	0.28
(1,846)	1:28:A:LEU:HD21	1:29:A:ASN:H	2	0.28
(1,846)	1:28:A:LEU:HD22	1:29:A:ASN:H	2	0.28
(1,846)	1:28:A:LEU:HD23	1:29:A:ASN:H	2	0.28
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	1	0.28
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	3	0.28
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	2	0.28
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	16	0.28
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE1	14	0.28
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE2	14	0.28
(1,747)	1:24:A:ILE:H	1:24:A:ILE:HG12	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	12	0.28
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	19	0.28
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	19	0.28
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	19	0.28
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	6	0.28
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	6	0.28
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	6	0.28
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	9	0.28
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	7	0.28
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	14	0.28
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	16	0.28
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	10	0.28
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	10	0.28
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	9	0.28
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	5	0.28
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	12	0.28
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	4	0.28
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	8	0.28
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	19	0.28
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	11	0.28
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	11	0.28
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	11	0.28
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	19	0.28
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	5	0.28
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	5	0.28
(1,148)	1:74:A:VAL:HG11	1:89:A:SER:H	3	0.28
(1,148)	1:74:A:VAL:HG12	1:89:A:SER:H	3	0.28
(1,148)	1:74:A:VAL:HG13	1:89:A:SER:H	3	0.28
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	1	0.28
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	19	0.27
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	19	0.27
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	19	0.27
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	19	0.27
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB2	12	0.27
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB3	12	0.27
(1,2481)	1:92:A:LYS:HE2	1:93:A:GLY:H	3	0.27
(1,2481)	1:92:A:LYS:HE3	1:93:A:GLY:H	3	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	3	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	3	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	3	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	3	0.27
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	3	0.27
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	3	0.27
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	10	0.27
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	10	0.27
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	9	0.27
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	9	0.27
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	5	0.27
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	5	0.27
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	5	0.27
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	5	0.27
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	13	0.27
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	13	0.27
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	12	0.27
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	12	0.27
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	1	0.27
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	1	0.27
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	7	0.27
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	7	0.27
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	11	0.27
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	11	0.27
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	20	0.27
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	20	0.27
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	20	0.27
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	20	0.27
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	9	0.27
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	9	0.27
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	8	0.27
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	8	0.27
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	9	0.27
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	9	0.27
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	10	0.27
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	10	0.27
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	13	0.27
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	13	0.27
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	17	0.27
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	17	0.27
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	15	0.27
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	13	0.27
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	13	0.27
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA2	17	0.27
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA3	17	0.27
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA2	17	0.27
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA3	17	0.27
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA2	17	0.27
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA3	17	0.27
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	15	0.27
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	15	0.27
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD11	1	0.27
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD12	1	0.27
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD13	1	0.27
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD11	1	0.27
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD12	1	0.27
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD13	1	0.27
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	1	0.27
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	1	0.27
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	1	0.27
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	1	0.27
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	1	0.27
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	1	0.27
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	7	0.27
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	7	0.27
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	7	0.27
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	7	0.27
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	1	0.27
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	1	0.27
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	1	0.27
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	1	0.27
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	1	0.27
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	1	0.27
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	1	0.27
(1,2055)	1:16:A:LEU:HD11	1:17:A:THR:HA	18	0.27
(1,2055)	1:16:A:LEU:HD12	1:17:A:THR:HA	18	0.27
(1,2055)	1:16:A:LEU:HD13	1:17:A:THR:HA	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2055)	1:16:A:LEU:HD21	1:17:A:THR:HA	18	0.27
(1,2055)	1:16:A:LEU:HD22	1:17:A:THR:HA	18	0.27
(1,2055)	1:16:A:LEU:HD23	1:17:A:THR:HA	18	0.27
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	2	0.27
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	2	0.27
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	2	0.27
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	2	0.27
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	2	0.27
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	2	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	16	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	16	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	16	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	16	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	16	0.27
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	16	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	2	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	2	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	2	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	2	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	2	0.27
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	2	0.27
(1,2015)	1:8:A:LEU:HD11	1:9:A:PRO:HD3	17	0.27
(1,2015)	1:8:A:LEU:HD12	1:9:A:PRO:HD3	17	0.27
(1,2015)	1:8:A:LEU:HD13	1:9:A:PRO:HD3	17	0.27
(1,2015)	1:8:A:LEU:HD21	1:9:A:PRO:HD3	17	0.27
(1,2015)	1:8:A:LEU:HD22	1:9:A:PRO:HD3	17	0.27
(1,2015)	1:8:A:LEU:HD23	1:9:A:PRO:HD3	17	0.27
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	18	0.27
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	18	0.27
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	2	0.27
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	2	0.27
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	2	0.27
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	2	0.27
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	2	0.27
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	2	0.27
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	14	0.27
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	14	0.27
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	14	0.27
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	14	0.27
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	14	0.27
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	14	0.27
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	2	0.27
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	2	0.27
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	2	0.27
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	18	0.27
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	18	0.27
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	18	0.27
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	16	0.27
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	12	0.27
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	19	0.27
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	19	0.27
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	19	0.27
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	19	0.27
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	19	0.27
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	19	0.27
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	2	0.27
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	2	0.27
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	14	0.27
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	9	0.27
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	20	0.27
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	8	0.27
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	8	0.27
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	8	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	4	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	4	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	4	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	14	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	14	0.27
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	14	0.27
(1,1325)	1:60:A:ARG:H	1:60:A:ARG:HD2	12	0.27
(1,1217)	1:105:A:ILE:HD11	1:114:A:ASP:HB3	13	0.27
(1,1217)	1:105:A:ILE:HD12	1:114:A:ASP:HB3	13	0.27
(1,1217)	1:105:A:ILE:HD13	1:114:A:ASP:HB3	13	0.27
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	4	0.27
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	19	0.27
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	19	0.27
(1,1123)	1:25:A:GLY:H	1:45:A:CYS:HA	16	0.27
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	5	0.27
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	5	0.27
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	5	0.27
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	8	0.27
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	8	0.27
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:95:A:ARG:HB2	1:121:A:ASP:HB3	2	0.27
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	5	0.27
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	5	0.27
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	5	0.27
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	11	0.27
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	11	0.27
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	11	0.27
(1,999)	1:61:A:LYS:HE2	1:111:A:VAL:HG21	15	0.27
(1,999)	1:61:A:LYS:HE2	1:111:A:VAL:HG22	15	0.27
(1,999)	1:61:A:LYS:HE2	1:111:A:VAL:HG23	15	0.27
(1,943)	1:46:A:LEU:H	1:51:A:TRP:H	14	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	4	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	4	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	4	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	7	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	7	0.27
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	7	0.27
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	7	0.27
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	16	0.27
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	2	0.27
(1,855)	1:34:A:PRO:HA	1:35:A:GLY:H	4	0.27
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	18	0.27
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	8	0.27
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	2	0.27
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	14	0.27
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	11	0.27
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	11	0.27
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	7	0.27
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	7	0.27
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	7	0.27
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	3	0.27
(1,637)	1:26:A:THR:HB	1:45:A:CYS:H	10	0.27
(1,628)	1:77:A:ILE:H	1:86:A:ILE:HB	19	0.27
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	2	0.27
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	7	0.27
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	7	0.27
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	7	0.27
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	19	0.27
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	20	0.27
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	10	0.27
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	11	0.27
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	12	0.27
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	17	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	10	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	10	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	11	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	11	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	16	0.27
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	16	0.27
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	19	0.27
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	4	0.27
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	17	0.27
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	8	0.27
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	4	0.27
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	4	0.27
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	4	0.27
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	6	0.27
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	6	0.27
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	6	0.27
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	17	0.27
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	17	0.27
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	17	0.27
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	20	0.26
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	20	0.26
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	20	0.26
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	20	0.26
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	8	0.26
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	8	0.26
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	8	0.26
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	8	0.26
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	8	0.26
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	8	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	3	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	3	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	3	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	3	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	3	0.26
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	3	0.26
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	11	0.26
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	11	0.26
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	12	0.26
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	12	0.26
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	12	0.26
(1,2419)	1:81:A:GLN:HB2	1:82:A:PHE:HB2	1	0.26
(1,2419)	1:81:A:GLN:HB3	1:82:A:PHE:HB2	1	0.26
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	9	0.26
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	9	0.26
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	2	0.26
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	2	0.26
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	3	0.26
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	3	0.26
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	1	0.26
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	1	0.26
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	8	0.26
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	8	0.26
(1,2267)	1:61:A:LYS:HG2	1:62:A:SER:HA	11	0.26
(1,2267)	1:61:A:LYS:HG3	1:62:A:SER:HA	11	0.26
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	13	0.26
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	13	0.26
(1,2243)	1:60:A:ARG:HG2	1:82:A:PHE:H	8	0.26
(1,2243)	1:60:A:ARG:HG3	1:82:A:PHE:H	8	0.26
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	5	0.26
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	5	0.26
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	11	0.26
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	11	0.26
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	13	0.26
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	13	0.26
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	14	0.26
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	14	0.26
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	14	0.26
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	14	0.26
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	14	0.26
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	14	0.26
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	8	0.26
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	8	0.26
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	2	0.26
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	2	0.26
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	2	0.26
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	2	0.26
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	20	0.26
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	20	0.26
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	6	0.26
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	6	0.26
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	6	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	12	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	14	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	14	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	14	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	14	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	14	0.26
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	14	0.26
(1,2027)	1:8:A:LEU:HD11	1:54:A:ALA:HA	20	0.26
(1,2027)	1:8:A:LEU:HD12	1:54:A:ALA:HA	20	0.26
(1,2027)	1:8:A:LEU:HD13	1:54:A:ALA:HA	20	0.26
(1,2027)	1:8:A:LEU:HD21	1:54:A:ALA:HA	20	0.26
(1,2027)	1:8:A:LEU:HD22	1:54:A:ALA:HA	20	0.26
(1,2027)	1:8:A:LEU:HD23	1:54:A:ALA:HA	20	0.26
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	12	0.26
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	12	0.26
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	17	0.26
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	17	0.26
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	4	0.26
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	4	0.26
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	4	0.26
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	4	0.26
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	4	0.26
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	4	0.26
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	12	0.26
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD11	15	0.26
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD12	15	0.26
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD13	15	0.26
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	19	0.26
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	19	0.26
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	19	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	19	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	19	0.26
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	19	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	19	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	19	0.26
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	7	0.26
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	15	0.26
(1,1687)	1:90:A:CYS:HB3	1:120:A:CYS:HA	14	0.26
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	9	0.26
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	9	0.26
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	4	0.26
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	4	0.26
(1,1553)	1:96:A:LEU:HD21	1:119:A:ILE:H	15	0.26
(1,1553)	1:96:A:LEU:HD22	1:119:A:ILE:H	15	0.26
(1,1553)	1:96:A:LEU:HD23	1:119:A:ILE:H	15	0.26
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	10	0.26
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	13	0.26
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	13	0.26
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	13	0.26
(1,1463)	1:96:A:LEU:HG	1:119:A:ILE:H	15	0.26
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	4	0.26
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	7	0.26
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	10	0.26
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	8	0.26
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	20	0.26
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	7	0.26
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	7	0.26
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	7	0.26
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	9	0.26
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	8	0.26
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	8	0.26
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	8	0.26
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	18	0.26
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	18	0.26
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	18	0.26
(1,1129)	1:122:A:ARG:H	1:122:A:ARG:HB3	16	0.26
(1,1096)	1:17:A:THR:HG21	1:19:A:GLU:HG3	15	0.26
(1,1096)	1:17:A:THR:HG22	1:19:A:GLU:HG3	15	0.26
(1,1096)	1:17:A:THR:HG23	1:19:A:GLU:HG3	15	0.26
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	15	0.26
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	15	0.26
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	15	0.26
(1,952)	1:107:A:SER:H	1:110:A:THR:H	7	0.26
(1,952)	1:107:A:SER:H	1:110:A:THR:H	17	0.26
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	6	0.26
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	6	0.26
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	2	0.26
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	15	0.26
(1,771)	1:51:A:TRP:H	1:51:A:TRP:HB2	16	0.26
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	8	0.26
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	11	0.26
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	20	0.26
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	20	0.26
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	20	0.26
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	18	0.26
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	15	0.26
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	16	0.26
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	7	0.26
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	13	0.26
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	1	0.26
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	20	0.26
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	20	0.26
(1,495)	1:96:A:LEU:H	1:120:A:CYS:HA	2	0.26
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	7	0.26
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	5	0.26
(1,415)	1:55:A:LYS:HA	1:57:A:ARG:H	7	0.26
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	15	0.26
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	4	0.26
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	14	0.26
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	1	0.26
(1,360)	1:105:A:ILE:H	1:114:A:ASP:HA	2	0.26
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	19	0.26
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	2	0.26
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	6	0.26
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	6	0.26
(1,150)	1:92:A:LYS:HB2	1:93:A:GLY:H	15	0.26
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	1	0.26
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	18	0.26
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	18	0.26
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	9	0.26
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	2	0.26
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	4	0.26
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	2	0.26
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	2	0.26
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	2	0.26
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB2	7	0.25
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB3	7	0.25
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	11	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	10	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	10	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	10	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	10	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	10	0.25
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	10	0.25
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	10	0.25
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	15	0.25
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	15	0.25
(1,2395)	1:76:A:VAL:HG11	1:113:A:TRP:HZ2	1	0.25
(1,2395)	1:76:A:VAL:HG12	1:113:A:TRP:HZ2	1	0.25
(1,2395)	1:76:A:VAL:HG13	1:113:A:TRP:HZ2	1	0.25
(1,2395)	1:76:A:VAL:HG21	1:113:A:TRP:HZ2	1	0.25
(1,2395)	1:76:A:VAL:HG22	1:113:A:TRP:HZ2	1	0.25
(1,2395)	1:76:A:VAL:HG23	1:113:A:TRP:HZ2	1	0.25
(1,2363)	1:73:A:MET:HG2	1:90:A:CYS:HA	12	0.25
(1,2363)	1:73:A:MET:HG3	1:90:A:CYS:HA	12	0.25
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	8	0.25
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	8	0.25
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	7	0.25
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	7	0.25
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	1	0.25
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	1	0.25
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	14	0.25
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	14	0.25
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	12	0.25
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	12	0.25
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	19	0.25
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	19	0.25
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	19	0.25
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	19	0.25
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	8	0.25
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	8	0.25
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	8	0.25
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	8	0.25
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	5	0.25
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	2	0.25
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	2	0.25
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	5	0.25
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	5	0.25
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	5	0.25
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	7	0.25
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	7	0.25
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	7	0.25
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	7	0.25
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	7	0.25
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	7	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	9	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	9	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	9	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	9	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	9	0.25
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	9	0.25
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	9	0.25
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	19	0.25
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	19	0.25
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	19	0.25
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	19	0.25
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	19	0.25
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	19	0.25
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	19	0.25
(1,2055)	1:16:A:LEU:HD11	1:17:A:THR:HA	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2055)	1:16:A:LEU:HD12	1:17:A:THR:HA	15	0.25
(1,2055)	1:16:A:LEU:HD13	1:17:A:THR:HA	15	0.25
(1,2055)	1:16:A:LEU:HD21	1:17:A:THR:HA	15	0.25
(1,2055)	1:16:A:LEU:HD22	1:17:A:THR:HA	15	0.25
(1,2055)	1:16:A:LEU:HD23	1:17:A:THR:HA	15	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	4	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	11	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	11	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	11	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	11	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	11	0.25
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	11	0.25
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	7	0.25
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	7	0.25
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	12	0.25
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	12	0.25
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	12	0.25
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	12	0.25
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	12	0.25
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	12	0.25
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	3	0.25
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	17	0.25
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	4	0.25
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	4	0.25
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	4	0.25
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	4	0.25
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	4	0.25
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	4	0.25
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	4	0.25
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	4	0.25
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	4	0.25
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	15	0.25
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	15	0.25
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	10	0.25
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	10	0.25
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	10	0.25
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	16	0.25
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	16	0.25
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	3	0.25
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	3	0.25
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	3	0.25
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	16	0.25
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	2	0.25
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	6	0.25
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	6	0.25
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	6	0.25
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	6	0.25
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	6	0.25
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	6	0.25
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	13	0.25
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	13	0.25
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	11	0.25
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	10	0.25
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	10	0.25
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	10	0.25
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	17	0.25
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	17	0.25
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	17	0.25
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	7	0.25
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	7	0.25
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	7	0.25
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	16	0.25
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	16	0.25
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	16	0.25
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD1	5	0.25
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD2	5	0.25
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	18	0.25
(1,1303)	1:119:A:ILE:HG12	1:120:A:CYS:H	14	0.25
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD1	14	0.25
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD2	14	0.25
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD1	14	0.25
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD2	14	0.25
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD1	14	0.25
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD2	14	0.25
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	8	0.25
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	8	0.25
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	7	0.25
(1,1129)	1:122:A:ARG:H	1:122:A:ARG:HB3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	4	0.25
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	4	0.25
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	4	0.25
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	14	0.25
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD11	17	0.25
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD12	17	0.25
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD13	17	0.25
(1,931)	1:65:A:ASN:HD22	1:67:A:PRO:HG2	14	0.25
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	17	0.25
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	17	0.25
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	5	0.25
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	5	0.25
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	5	0.25
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	17	0.25
(1,892)	1:3:A:ASN:HD21	1:4:A:ALA:H	8	0.25
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	15	0.25
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	18	0.25
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	6	0.25
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	6	0.25
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	16	0.25
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	16	0.25
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	16	0.25
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	3	0.25
(1,667)	1:1:A:GLN:HB2	1:22:A:PHE:H	6	0.25
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	19	0.25
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	19	0.25
(1,644)	1:75:A:HIS:HA	1:76:A:VAL:H	9	0.25
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	7	0.25
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	7	0.25
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	12	0.25
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	14	0.25
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	8	0.25
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	2	0.25
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	2	0.25
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	2	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	9	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	9	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	10	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	10	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	18	0.25
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	18	0.25
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	8	0.25
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	18	0.25
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	20	0.25
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	5	0.25
(1,2546)	1:104:A:CYS:HA	1:114:A:ASP:HB2	17	0.24
(1,2546)	1:104:A:CYS:HA	1:114:A:ASP:HB3	17	0.24
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	19	0.24
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	19	0.24
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	4	0.24
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	4	0.24
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	4	0.24
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	4	0.24
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	15	0.24
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	15	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	15	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	15	0.24
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	20	0.24
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	20	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	20	0.24
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	20	0.24
(1,2428)	1:84:A:SER:HB2	1:104:A:CYS:H	13	0.24
(1,2428)	1:84:A:SER:HB3	1:104:A:CYS:H	13	0.24
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE2	10	0.24
(1,2406)	1:78:A:LYS:HA	1:78:A:LYS:HE3	10	0.24
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	4	0.24
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	4	0.24
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB2	12	0.24
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB3	12	0.24
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	6	0.24
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	6	0.24
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	20	0.24
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	1:64:A:ARG:HD2	1:65:A:ASN:H	11	0.24
(1,2303)	1:64:A:ARG:HD3	1:65:A:ASN:H	11	0.24
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	2	0.24
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	2	0.24
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	9	0.24
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	9	0.24
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	9	0.24
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	9	0.24
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	1	0.24
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	1	0.24
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	12	0.24
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	12	0.24
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	13	0.24
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	13	0.24
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	8	0.24
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	8	0.24
(1,2209)	1:55:A:LYS:HG2	1:56:A:ASP:HA	8	0.24
(1,2209)	1:55:A:LYS:HG3	1:56:A:ASP:HA	8	0.24
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	1	0.24
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	1	0.24
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	11	0.24
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	11	0.24
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	10	0.24
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	10	0.24
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB2	11	0.24
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB3	11	0.24
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	16	0.24
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	16	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	14	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	14	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	14	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	14	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	14	0.24
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	14	0.24
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	14	0.24
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	20	0.24
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	20	0.24
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	20	0.24
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	20	0.24
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	20	0.24
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	4	0.24
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	4	0.24
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	1	0.24
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	1	0.24
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	16	0.24
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	16	0.24
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	10	0.24
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	8	0.24
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	8	0.24
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	8	0.24
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG2	3	0.24
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG3	3	0.24
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	19	0.24
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	19	0.24
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	19	0.24
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	2	0.24
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	2	0.24
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	2	0.24
(1,1763)	1:16:A:LEU:HA	1:20:A:PHE:HB2	18	0.24
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	2	0.24
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	13	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	2	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	2	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	2	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	14	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	14	0.24
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	14	0.24
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	6	0.24
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	6	0.24
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	6	0.24
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	20	0.24
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	11	0.24
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	8	0.24
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	8	0.24
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	10	0.24
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	10	0.24
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE1	8	0.24
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:71:A:ASN:HB3	1:73:A:MET:HE3	8	0.24
(1,1553)	1:96:A:LEU:HD21	1:119:A:ILE:H	4	0.24
(1,1553)	1:96:A:LEU:HD22	1:119:A:ILE:H	4	0.24
(1,1553)	1:96:A:LEU:HD23	1:119:A:ILE:H	4	0.24
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	19	0.24
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	19	0.24
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	19	0.24
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	16	0.24
(1,1479)	1:110:A:THR:HG21	1:112:A:ILE:HB	19	0.24
(1,1479)	1:110:A:THR:HG22	1:112:A:ILE:HB	19	0.24
(1,1479)	1:110:A:THR:HG23	1:112:A:ILE:HB	19	0.24
(1,1462)	1:96:A:LEU:HG	1:119:A:ILE:HB	14	0.24
(1,1461)	1:4:A:ALA:H	1:20:A:PHE:HA	2	0.24
(1,1452)	1:2:A:CYS:HB2	1:5:A:PRO:HA	8	0.24
(1,1355)	1:13:A:PRO:HB2	1:30:A:TYR:HA	1	0.24
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	14	0.24
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	14	0.24
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	14	0.24
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	15	0.24
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	19	0.24
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	2	0.24
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	2	0.24
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	2	0.24
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	14	0.24
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	14	0.24
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	12	0.24
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	17	0.24
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	17	0.24
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	4	0.24
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	4	0.24
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	4	0.24
(1,952)	1:107:A:SER:H	1:110:A:THR:H	15	0.24
(1,952)	1:107:A:SER:H	1:110:A:THR:H	19	0.24
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	15	0.24
(1,927)	1:65:A:ASN:HD21	1:68:A:ASP:HA	12	0.24
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD1	13	0.24
(1,909)	1:15:A:GLN:HE22	1:30:A:TYR:HD2	13	0.24
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	14	0.24
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	14	0.24
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	16	0.24
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	5	0.24
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	12	0.24
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	12	0.24
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	5	0.24
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	11	0.24
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	12	0.24
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	12	0.24
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	12	0.24
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	5	0.24
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	13	0.24
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	13	0.24
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	13	0.24
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	4	0.24
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	5	0.24
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	14	0.24
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	14	0.24
(1,649)	1:74:A:VAL:H	1:89:A:SER:H	13	0.24
(1,628)	1:77:A:ILE:H	1:86:A:ILE:HB	7	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	12	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	12	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	12	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	14	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	14	0.24
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	14	0.24
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	12	0.24
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	19	0.24
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	11	0.24
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	14	0.24
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	3	0.24
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	10	0.24
(1,213)	1:30:A:TYR:HD1	1:43:A:ILE:H	12	0.24
(1,213)	1:30:A:TYR:HD2	1:43:A:ILE:H	12	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	4	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	4	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	4	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	5	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	5	0.24
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	5	0.24
(1,183)	1:99:A:SER:H	1:119:A:ILE:H	5	0.24
(1,88)	1:96:A:LEU:HD11	1:97:A:ILE:H	13	0.24
(1,88)	1:96:A:LEU:HD12	1:97:A:ILE:H	13	0.24
(1,88)	1:96:A:LEU:HD13	1:97:A:ILE:H	13	0.24
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	3	0.24
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	7	0.24
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	15	0.24
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	15	0.24
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	15	0.24
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG11	4	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG12	4	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG13	4	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG11	4	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG12	4	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG13	4	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG11	5	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG12	5	0.23
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG13	5	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG11	5	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG12	5	0.23
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG13	5	0.23
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	3	0.23
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	3	0.23
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	3	0.23
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	3	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD11	13	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD12	13	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD13	13	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD21	13	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD22	13	0.23
(1,2496)	1:96:A:LEU:HA	1:96:A:LEU:HD23	13	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	19	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	19	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	19	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	19	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	19	0.23
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	19	0.23
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	19	0.23
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB2	1	0.23
(1,2431)	1:85:A:GLN:H	1:104:A:CYS:HB3	1	0.23
(1,2428)	1:84:A:SER:HB2	1:104:A:CYS:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2428)	1:84:A:SER:HB3	1:104:A:CYS:H	6	0.23
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE1	11	0.23
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE2	11	0.23
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE3	11	0.23
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE1	11	0.23
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE2	11	0.23
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE3	11	0.23
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	6	0.23
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	6	0.23
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	6	0.23
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	6	0.23
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	11	0.23
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	11	0.23
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	12	0.23
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	12	0.23
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	5	0.23
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	5	0.23
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	16	0.23
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	16	0.23
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	7	0.23
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	7	0.23
(1,2283)	1:62:A:SER:HB2	1:64:A:ARG:HB3	9	0.23
(1,2283)	1:62:A:SER:HB3	1:64:A:ARG:HB3	9	0.23
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	5	0.23
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	5	0.23
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	3	0.23
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	3	0.23
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	13	0.23
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	13	0.23
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	3	0.23
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	3	0.23
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	3	0.23
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	3	0.23
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	3	0.23
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	3	0.23
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	4	0.23
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	4	0.23
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	9	0.23
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	9	0.23
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	9	0.23
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	9	0.23
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	9	0.23
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	17	0.23
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	18	0.23
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	18	0.23
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	18	0.23
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	18	0.23
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	18	0.23
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	18	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	13	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	13	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	13	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	13	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	13	0.23
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	13	0.23
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	13	0.23
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG2	17	0.23
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG3	17	0.23
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	16	0.23
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	16	0.23
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	16	0.23
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	16	0.23
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	16	0.23
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	16	0.23
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	16	0.23
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	18	0.23
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	18	0.23
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	18	0.23
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	18	0.23
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	18	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	3	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	3	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	19	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	19	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	20	0.23
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	20	0.23
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	11	0.23
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	11	0.23
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	18	0.23
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	18	0.23
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	18	0.23
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	18	0.23
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	18	0.23
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	18	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	8	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	8	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	8	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	8	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	8	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	8	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	8	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	8	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	8	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	16	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	16	0.23
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	16	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	16	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	16	0.23
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	16	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	16	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	16	0.23
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	16	0.23
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	10	0.23
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	6	0.23
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG21	10	0.23
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG22	10	0.23
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG23	10	0.23
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	15	0.23
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	15	0.23
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	12	0.23
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	12	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	2	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	2	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	2	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	2	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	2	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	2	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	4	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	4	0.23
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	4	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	4	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	4	0.23
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	4	0.23
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	4	0.23
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	6	0.23
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	6	0.23
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	13	0.23
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	10	0.23
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	10	0.23
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	1	0.23
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	1	0.23
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	19	0.23
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	19	0.23
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	19	0.23
(1,1521)	1:91:A:THR:HG21	1:92:A:LYS:HB3	5	0.23
(1,1521)	1:91:A:THR:HG22	1:92:A:LYS:HB3	5	0.23
(1,1521)	1:91:A:THR:HG23	1:92:A:LYS:HB3	5	0.23
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	14	0.23
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	14	0.23
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	14	0.23
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	12	0.23
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	12	0.23
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	12	0.23
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	4	0.23
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	4	0.23
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	4	0.23
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	7	0.23
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	7	0.23
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	7	0.23
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	12	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	8	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	8	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	8	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	10	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	10	0.23
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	10	0.23
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	12	0.23
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	17	0.23
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	17	0.23
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	17	0.23
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	4	0.23
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	4	0.23
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	14	0.23
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	14	0.23
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	13	0.23
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	13	0.23
(1,1097)	1:17:A:THR:HG21	1:19:A:GLU:HG2	18	0.23
(1,1097)	1:17:A:THR:HG22	1:19:A:GLU:HG2	18	0.23
(1,1097)	1:17:A:THR:HG23	1:19:A:GLU:HG2	18	0.23
(1,1035)	1:2:A:CYS:HB2	1:4:A:ALA:HB1	16	0.23
(1,1035)	1:2:A:CYS:HB2	1:4:A:ALA:HB2	16	0.23
(1,1035)	1:2:A:CYS:HB2	1:4:A:ALA:HB3	16	0.23
(1,1027)	1:80:A:ILE:H	1:80:A:ILE:HD11	2	0.23
(1,1027)	1:80:A:ILE:H	1:80:A:ILE:HD12	2	0.23
(1,1027)	1:80:A:ILE:H	1:80:A:ILE:HD13	2	0.23
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	15	0.23
(1,862)	1:13:A:PRO:HA	1:31:A:GLU:H	20	0.23
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	5	0.23
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	3	0.23
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	7	0.23
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	13	0.23
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE1	16	0.23
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE2	16	0.23
(1,795)	1:18:A:ASP:H	1:19:A:GLU:HG3	15	0.23
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	16	0.23
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	7	0.23
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	7	0.23
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	17	0.23
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	17	0.23
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD1	14	0.23
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	3	0.23
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	9	0.23
(1,667)	1:1:A:GLN:HB2	1:22:A:PHE:H	16	0.23
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD1	7	0.23
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD2	7	0.23
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	10	0.23
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	4	0.23
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	11	0.23
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	8	0.23
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	3	0.23
(1,495)	1:96:A:LEU:H	1:120:A:CYS:HA	15	0.23
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	17	0.23
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	6	0.23
(1,465)	1:109:A:ASP:H	1:110:A:THR:HG21	9	0.23
(1,465)	1:109:A:ASP:H	1:110:A:THR:HG22	9	0.23
(1,465)	1:109:A:ASP:H	1:110:A:THR:HG23	9	0.23
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	9	0.23
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	4	0.23
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	5	0.23
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	16	0.23
(1,171)	1:14:A:THR:H	1:15:A:GLN:HB2	18	0.23
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	6	0.23
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	6	0.23
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	13	0.23
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	15	0.23
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	19	0.23
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	19	0.23
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	19	0.23
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	4	0.23
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	4	0.23
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	4	0.23
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB2	20	0.22
(1,2578)	1:121:A:ASP:HA	1:122:A:ARG:HB3	20	0.22
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	1	0.22
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	1	0.22
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	1	0.22
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	1	0.22
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	1	0.22
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	1	0.22
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	15	0.22
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	15	0.22
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	15	0.22
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB2	9	0.22
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB3	9	0.22
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	12	0.22
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	12	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	6	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	6	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	6	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	6	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	6	0.22
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	6	0.22
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	6	0.22
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	7	0.22
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	7	0.22
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	7	0.22
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	7	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	2	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	2	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	11	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	11	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	17	0.22
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	17	0.22
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	14	0.22
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	14	0.22
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG21	14	0.22
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG22	14	0.22
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG23	14	0.22
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG21	14	0.22
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG22	14	0.22
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG23	14	0.22
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	4	0.22
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	4	0.22
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	14	0.22
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	14	0.22
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	16	0.22
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	16	0.22
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	6	0.22
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	6	0.22
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	6	0.22
(1,2209)	1:55:A:LYS:HG2	1:56:A:ASP:HA	12	0.22
(1,2209)	1:55:A:LYS:HG3	1:56:A:ASP:HA	12	0.22
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	11	0.22
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	11	0.22
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	5	0.22
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	5	0.22
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	5	0.22
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	5	0.22
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	5	0.22
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	5	0.22
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	4	0.22
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	4	0.22
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	4	0.22
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	4	0.22
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	1	0.22
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	1	0.22
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	1	0.22
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	1	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	20	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	20	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	20	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	20	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	20	0.22
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	20	0.22
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	20	0.22
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	13	0.22
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	13	0.22
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	13	0.22
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	13	0.22
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	13	0.22
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	13	0.22
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	13	0.22
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	13	0.22
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	13	0.22
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	13	0.22
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	13	0.22
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG2	18	0.22
(1,1991)	1:5:A:PRO:HA	1:6:A:GLU:HG3	18	0.22
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	18	0.22
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	18	0.22
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	8	0.22
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	8	0.22
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE1	11	0.22
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE2	11	0.22
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	20	0.22
(1,1894)	1:15:A:GLN:HB2	1:28:A:LEU:HD21	2	0.22
(1,1894)	1:15:A:GLN:HB2	1:28:A:LEU:HD22	2	0.22
(1,1894)	1:15:A:GLN:HB2	1:28:A:LEU:HD23	2	0.22
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	2	0.22
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	19	0.22
(1,1814)	1:73:A:MET:HE1	1:92:A:LYS:H	13	0.22
(1,1814)	1:73:A:MET:HE2	1:92:A:LYS:H	13	0.22
(1,1814)	1:73:A:MET:HE3	1:92:A:LYS:H	13	0.22
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	8	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	3	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	3	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	3	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	16	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	16	0.22
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	16	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	14	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	14	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	14	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	19	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	19	0.22
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	19	0.22
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	11	0.22
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	11	0.22
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	11	0.22
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	2	0.22
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	2	0.22
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	2	0.22
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	16	0.22
(1,1629)	1:87:A:LYS:HA	1:87:A:LYS:HG3	3	0.22
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	8	0.22
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	8	0.22
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	11	0.22
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	11	0.22
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	11	0.22
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	16	0.22
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	16	0.22
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	16	0.22
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	6	0.22
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	6	0.22
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	4	0.22
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	4	0.22
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	4	0.22
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	7	0.22
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	7	0.22
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	7	0.22
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	1	0.22
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	1	0.22
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	1	0.22
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	16	0.22
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	16	0.22
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	16	0.22
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	1	0.22
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	14	0.22
(1,1452)	1:2:A:CYS:HB2	1:5:A:PRO:HA	17	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	7	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	7	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	7	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	15	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	15	0.22
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	15	0.22
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	18	0.22
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	18	0.22
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	18	0.22
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	18	0.22
(1,1326)	1:60:A:ARG:HD2	1:82:A:PHE:H	6	0.22
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	15	0.22
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	15	0.22
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	15	0.22
(1,1272)	1:14:A:THR:HG21	1:29:A:ASN:HB2	17	0.22
(1,1272)	1:14:A:THR:HG22	1:29:A:ASN:HB2	17	0.22
(1,1272)	1:14:A:THR:HG23	1:29:A:ASN:HB2	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	17	0.22
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	17	0.22
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	17	0.22
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	5	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD11	2	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD12	2	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD13	2	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD11	15	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD12	15	0.22
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD13	15	0.22
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD11	19	0.22
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD12	19	0.22
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD13	19	0.22
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	10	0.22
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	10	0.22
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	10	0.22
(1,952)	1:107:A:SER:H	1:110:A:THR:H	2	0.22
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	7	0.22
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	7	0.22
(1,906)	1:1:A:GLN:HB2	1:1:A:GLN:HE21	10	0.22
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	10	0.22
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	10	0.22
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	10	0.22
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	17	0.22
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	1	0.22
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	1	0.22
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	19	0.22
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	19	0.22
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	10	0.22
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	11	0.22
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	12	0.22
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	14	0.22
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	19	0.22
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	9	0.22
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	7	0.22
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	7	0.22
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	4	0.22
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	8	0.22
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	4	0.22
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	8	0.22
(1,799)	1:19:A:GLU:H	1:20:A:PHE:HD1	18	0.22
(1,799)	1:19:A:GLU:H	1:20:A:PHE:HD2	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	8	0.22
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	8	0.22
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	14	0.22
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	5	0.22
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	5	0.22
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	5	0.22
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	16	0.22
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	19	0.22
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	9	0.22
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	17	0.22
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	17	0.22
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	17	0.22
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	20	0.22
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	20	0.22
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	20	0.22
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	9	0.22
(1,583)	1:26:A:THR:H	1:51:A:TRP:HH2	12	0.22
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	17	0.22
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	9	0.22
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	18	0.22
(1,555)	1:55:A:LYS:HA	1:56:A:ASP:H	18	0.22
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	2	0.22
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	5	0.22
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	9	0.22
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB2	3	0.22
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB3	3	0.22
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	1	0.22
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	16	0.22
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	16	0.22
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	18	0.22
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	19	0.22
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	7	0.22
(1,263)	1:55:A:LYS:H	1:57:A:ARG:HD3	2	0.22
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	2	0.22
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	4	0.22
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	15	0.22
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	4	0.22
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	4	0.22
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	1	0.22
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	1	0.22
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	10	0.22
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	17	0.22
(1,41)	1:12:A:ARG:H	1:31:A:GLU:HB2	3	0.22
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	14	0.22
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	8	0.21
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	8	0.21
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	8	0.21
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	8	0.21
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	8	0.21
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	8	0.21
(1,2556)	1:107:A:SER:HB2	1:112:A:ILE:H	8	0.21
(1,2556)	1:107:A:SER:HB3	1:112:A:ILE:H	8	0.21
(1,2556)	1:107:A:SER:HB2	1:112:A:ILE:H	18	0.21
(1,2556)	1:107:A:SER:HB3	1:112:A:ILE:H	18	0.21
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	14	0.21
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	14	0.21
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	14	0.21
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	14	0.21
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	14	0.21
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	14	0.21
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	14	0.21
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	14	0.21
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	14	0.21
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	7	0.21
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	7	0.21
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	18	0.21
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	18	0.21
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	20	0.21
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	20	0.21
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	15	0.21
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	15	0.21
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE2	2	0.21
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE3	2	0.21
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	1	0.21
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	1	0.21
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	2	0.21
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	2	0.21
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	20	0.21
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	20	0.21
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	20	0.21
(1,2291)	1:63:A:CYS:HB2	1:81:A:GLN:HB2	17	0.21
(1,2291)	1:63:A:CYS:HB2	1:81:A:GLN:HB3	17	0.21
(1,2291)	1:63:A:CYS:HB3	1:81:A:GLN:HB2	17	0.21
(1,2291)	1:63:A:CYS:HB3	1:81:A:GLN:HB3	17	0.21
(1,2283)	1:62:A:SER:HB2	1:64:A:ARG:HB3	4	0.21
(1,2283)	1:62:A:SER:HB3	1:64:A:ARG:HB3	4	0.21
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	1	0.21
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	1	0.21
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	1	0.21
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	1	0.21
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE2	15	0.21
(1,2259)	1:61:A:LYS:H	1:61:A:LYS:HE3	15	0.21
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	18	0.21
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	18	0.21
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	2	0.21
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	2	0.21
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	11	0.21
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	11	0.21
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	11	0.21
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	11	0.21
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	9	0.21
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	9	0.21
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	9	0.21
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	9	0.21
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	9	0.21
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	9	0.21
(1,2161)	1:47:A:LYS:HB2	1:52:A:THR:HA	1	0.21
(1,2161)	1:47:A:LYS:HB3	1:52:A:THR:HA	1	0.21
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	10	0.21
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	10	0.21
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	10	0.21
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	10	0.21
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	10	0.21
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	10	0.21
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	5	0.21
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	5	0.21
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	5	0.21
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	5	0.21
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	5	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	4	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	4	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	4	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	4	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	5	0.21
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	5	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	5	0.21
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	5	0.21
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD2	3	0.21
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD3	3	0.21
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD2	3	0.21
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD3	3	0.21
(1,2127)	1:39:A:ARG:HA	1:39:A:ARG:HD2	9	0.21
(1,2127)	1:39:A:ARG:HA	1:39:A:ARG:HD3	9	0.21
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	12	0.21
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	12	0.21
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	12	0.21
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	12	0.21
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	12	0.21
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	12	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	15	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	15	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	15	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	15	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	15	0.21
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	15	0.21
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	15	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	11	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	11	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	11	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	11	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	11	0.21
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	11	0.21
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	1	0.21
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	1	0.21
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	1	0.21
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	1	0.21
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	1	0.21
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	17	0.21
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	17	0.21
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	4	0.21
(1,1897)	1:9:A:PRO:HB2	1:10:A:PHE:HD1	15	0.21
(1,1897)	1:9:A:PRO:HB2	1:10:A:PHE:HD2	15	0.21
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	14	0.21
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	15	0.21
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	1	0.21
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	1	0.21
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	1	0.21
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	1	0.21
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	1	0.21
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	1	0.21
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	14	0.21
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	14	0.21
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	14	0.21
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG21	4	0.21
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG22	4	0.21
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG23	4	0.21
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	6	0.21
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	6	0.21
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	6	0.21
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	6	0.21
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	6	0.21
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	6	0.21
(1,1763)	1:16:A:LEU:HA	1:20:A:PHE:HB2	7	0.21
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	3	0.21
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	3	0.21
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	3	0.21
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	10	0.21
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB1	13	0.21
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB2	13	0.21
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB3	13	0.21
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB1	13	0.21
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB2	13	0.21
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB3	13	0.21
(1,1697)	1:99:A:SER:HB3	1:115:A:GLN:HA	18	0.21
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	17	0.21
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	2	0.21
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	2	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	2	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	2	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	2	0.21
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	9	0.21
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	9	0.21
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	9	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	9	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	9	0.21
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	9	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	3	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	3	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	3	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	7	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	7	0.21
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	7	0.21
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	18	0.21
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	15	0.21
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	15	0.21
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	3	0.21
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	3	0.21
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	3	0.21
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	3	0.21
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	3	0.21
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	3	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	4	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	4	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	4	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	16	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	16	0.21
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	16	0.21
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	20	0.21
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	20	0.21
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	20	0.21
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	1	0.21
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	20	0.21
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	20	0.21
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	20	0.21
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD1	10	0.21
(1,1261)	1:73:A:MET:HE1	1:94:A:TYR:HD2	10	0.21
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD1	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1261)	1:73:A:MET:HE2	1:94:A:TYR:HD2	10	0.21
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD1	10	0.21
(1,1261)	1:73:A:MET:HE3	1:94:A:TYR:HD2	10	0.21
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	10	0.21
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	10	0.21
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	10	0.21
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	6	0.21
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	6	0.21
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	6	0.21
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	12	0.21
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD11	3	0.21
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD12	3	0.21
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD13	3	0.21
(1,1112)	1:33:A:ARG:H	1:36:A:TYR:HB3	7	0.21
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD11	18	0.21
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD12	18	0.21
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD13	18	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD11	18	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD12	18	0.21
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD13	18	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD11	18	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD12	18	0.21
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD13	18	0.21
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD11	8	0.21
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD12	8	0.21
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD13	8	0.21
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD11	8	0.21
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD12	8	0.21
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD13	8	0.21
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD11	8	0.21
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD12	8	0.21
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD13	8	0.21
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	3	0.21
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	3	0.21
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	3	0.21
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	11	0.21
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	11	0.21
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	11	0.21
(1,952)	1:107:A:SER:H	1:110:A:THR:H	4	0.21
(1,918)	1:13:A:PRO:HB2	1:15:A:GLN:HE21	11	0.21
(1,905)	1:1:A:GLN:HB2	1:1:A:GLN:HE22	4	0.21
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	17	0.21
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	17	0.21
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	1	0.21
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	15	0.21
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	5	0.21
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	6	0.21
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	20	0.21
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	1	0.21
(1,796)	1:18:A:ASP:H	1:19:A:GLU:HG2	1	0.21
(1,790)	1:16:A:LEU:H	1:28:A:LEU:HG	14	0.21
(1,780)	1:17:A:THR:H	1:19:A:GLU:HG3	14	0.21
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	6	0.21
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	1	0.21
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	1	0.21
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	1	0.21
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	1	0.21
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	5	0.21
(1,667)	1:1:A:GLN:HB2	1:22:A:PHE:H	12	0.21
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD1	11	0.21
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD2	11	0.21
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	13	0.21
(1,583)	1:26:A:THR:H	1:51:A:TRP:HH2	17	0.21
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	5	0.21
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	20	0.21
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	15	0.21
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	15	0.21
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	15	0.21
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	12	0.21
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	15	0.21
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	16	0.21
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	14	0.21
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	17	0.21
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	14	0.21
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	19	0.21
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	8	0.21
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	9	0.21
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	1	0.21
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	16	0.21
(1,204)	1:111:A:VAL:H	1:112:A:ILE:HG21	7	0.21
(1,204)	1:111:A:VAL:H	1:112:A:ILE:HG22	7	0.21
(1,204)	1:111:A:VAL:H	1:112:A:ILE:HG23	7	0.21
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	13	0.21
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	13	0.21
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	20	0.21
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	20	0.21
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	20	0.21
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	14	0.21
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	14	0.21
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	19	0.21
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	19	0.21
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	13	0.21
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	13	0.21
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	13	0.21
(1,83)	1:36:A:TYR:HE1	1:60:A:ARG:H	4	0.21
(1,83)	1:36:A:TYR:HE2	1:60:A:ARG:H	4	0.21
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	3	0.21
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	16	0.21
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	18	0.21
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	15	0.21
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	15	0.21
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	15	0.21
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	15	0.2
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	15	0.2
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	15	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	15	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	15	0.2
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	15	0.2
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	5	0.2
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	5	0.2
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	5	0.2
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	5	0.2
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	1	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	1	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	1	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	1	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	1	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	1	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	12	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	12	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	12	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	12	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	12	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	12	0.2
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	12	0.2
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB2	13	0.2
(1,2500)	1:96:A:LEU:HG	1:100:A:SER:HB3	13	0.2
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	8	0.2
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	8	0.2
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	11	0.2
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	11	0.2
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	20	0.2
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	20	0.2
(1,2461)	1:90:A:CYS:HB2	1:91:A:THR:H	13	0.2
(1,2461)	1:90:A:CYS:HB3	1:91:A:THR:H	13	0.2
(1,2461)	1:90:A:CYS:HB2	1:91:A:THR:H	14	0.2
(1,2461)	1:90:A:CYS:HB3	1:91:A:THR:H	14	0.2
(1,2388)	1:76:A:VAL:HG11	1:78:A:LYS:H	6	0.2
(1,2388)	1:76:A:VAL:HG12	1:78:A:LYS:H	6	0.2
(1,2388)	1:76:A:VAL:HG13	1:78:A:LYS:H	6	0.2
(1,2388)	1:76:A:VAL:HG21	1:78:A:LYS:H	6	0.2
(1,2388)	1:76:A:VAL:HG22	1:78:A:LYS:H	6	0.2
(1,2388)	1:76:A:VAL:HG23	1:78:A:LYS:H	6	0.2
(1,2387)	1:76:A:VAL:HG11	1:77:A:ILE:H	15	0.2
(1,2387)	1:76:A:VAL:HG12	1:77:A:ILE:H	15	0.2
(1,2387)	1:76:A:VAL:HG13	1:77:A:ILE:H	15	0.2
(1,2387)	1:76:A:VAL:HG21	1:77:A:ILE:H	15	0.2
(1,2387)	1:76:A:VAL:HG22	1:77:A:ILE:H	15	0.2
(1,2387)	1:76:A:VAL:HG23	1:77:A:ILE:H	15	0.2
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	11	0.2
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	11	0.2
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	12	0.2
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	12	0.2
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	13	0.2
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	13	0.2
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	13	0.2
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	18	0.2
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	18	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG11	12	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG12	12	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG13	12	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG21	12	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG22	12	0.2
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG23	12	0.2
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	15	0.2
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	15	0.2
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	1	0.2
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	1	0.2
(1,2242)	1:60:A:ARG:HG2	1:81:A:GLN:HE21	11	0.2
(1,2242)	1:60:A:ARG:HG3	1:81:A:GLN:HE21	11	0.2
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	4	0.2
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	4	0.2
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	7	0.2
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	7	0.2
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	10	0.2
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	10	0.2
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	14	0.2
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	14	0.2
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	19	0.2
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	19	0.2
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	12	0.2
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	12	0.2
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	12	0.2
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	12	0.2
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	12	0.2
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	12	0.2
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	12	0.2
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	12	0.2
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	12	0.2
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	12	0.2
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD2	2	0.2
(1,2130)	1:39:A:ARG:HB2	1:40:A:PRO:HD3	2	0.2
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD2	2	0.2
(1,2130)	1:39:A:ARG:HB3	1:40:A:PRO:HD3	2	0.2
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD2	19	0.2
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD3	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD2	19	0.2
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD3	19	0.2
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	3	0.2
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	3	0.2
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	3	0.2
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	3	0.2
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	3	0.2
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	3	0.2
(1,2055)	1:16:A:LEU:HD11	1:17:A:THR:HA	20	0.2
(1,2055)	1:16:A:LEU:HD12	1:17:A:THR:HA	20	0.2
(1,2055)	1:16:A:LEU:HD13	1:17:A:THR:HA	20	0.2
(1,2055)	1:16:A:LEU:HD21	1:17:A:THR:HA	20	0.2
(1,2055)	1:16:A:LEU:HD22	1:17:A:THR:HA	20	0.2
(1,2055)	1:16:A:LEU:HD23	1:17:A:THR:HA	20	0.2
(1,2054)	1:16:A:LEU:HD11	1:17:A:THR:H	10	0.2
(1,2054)	1:16:A:LEU:HD12	1:17:A:THR:H	10	0.2
(1,2054)	1:16:A:LEU:HD13	1:17:A:THR:H	10	0.2
(1,2054)	1:16:A:LEU:HD21	1:17:A:THR:H	10	0.2
(1,2054)	1:16:A:LEU:HD22	1:17:A:THR:H	10	0.2
(1,2054)	1:16:A:LEU:HD23	1:17:A:THR:H	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	10	0.2
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	10	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD11	2	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD12	2	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD13	2	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD21	2	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD22	2	0.2
(1,1995)	1:5:A:PRO:HD2	1:28:A:LEU:HD23	2	0.2
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	6	0.2
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	6	0.2
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	4	0.2
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	4	0.2
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	10	0.2
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	10	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	3	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	3	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	3	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	3	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	3	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	14	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	14	0.2
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	14	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	14	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	14	0.2
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	14	0.2
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	1	0.2
(1,1898)	1:15:A:GLN:HB3	1:15:A:GLN:HE22	20	0.2
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	4	0.2
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	4	0.2
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	4	0.2
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE1	18	0.2
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE2	18	0.2
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE3	18	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	15	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	15	0.2
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	15	0.2
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	1	0.2
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	1	0.2
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	1	0.2
(1,1757)	1:9:A:PRO:HA	1:11:A:ALA:HB1	19	0.2
(1,1757)	1:9:A:PRO:HA	1:11:A:ALA:HB2	19	0.2
(1,1757)	1:9:A:PRO:HA	1:11:A:ALA:HB3	19	0.2
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	11	0.2
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	11	0.2
(1,1736)	1:61:A:LYS:HB3	1:111:A:VAL:HA	12	0.2
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	3	0.2
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	11	0.2
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	11	0.2
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	11	0.2
(1,1700)	1:5:A:PRO:HD2	1:20:A:PHE:HB3	3	0.2
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	17	0.2
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	20	0.2
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	20	0.2
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	20	0.2
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	11	0.2
(1,1629)	1:87:A:LYS:HA	1:87:A:LYS:HG3	4	0.2
(1,1629)	1:87:A:LYS:HA	1:87:A:LYS:HG3	8	0.2
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	11	0.2
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	13	0.2
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	13	0.2
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	13	0.2
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	20	0.2
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	20	0.2
(1,1525)	1:16:A:LEU:HB2	1:28:A:LEU:HG	7	0.2
(1,1525)	1:16:A:LEU:HB3	1:28:A:LEU:HG	7	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	2	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	2	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	2	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	15	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	15	0.2
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	15	0.2
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	2	0.2
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	2	0.2
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	2	0.2
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	5	0.2
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	5	0.2
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	5	0.2
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	13	0.2
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	13	0.2
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	13	0.2
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	2	0.2
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	2	0.2
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	2	0.2
(1,1461)	1:4:A:ALA:H	1:20:A:PHE:HA	15	0.2
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	19	0.2
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	9	0.2
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	9	0.2
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	9	0.2
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	13	0.2
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	13	0.2
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	13	0.2
(1,1312)	1:96:A:LEU:HG	1:120:A:CYS:HA	18	0.2
(1,1271)	1:13:A:PRO:HA	1:14:A:THR:HG21	2	0.2
(1,1271)	1:13:A:PRO:HA	1:14:A:THR:HG22	2	0.2
(1,1271)	1:13:A:PRO:HA	1:14:A:THR:HG23	2	0.2
(1,1240)	1:4:A:ALA:HB1	1:51:A:TRP:HZ2	19	0.2
(1,1240)	1:4:A:ALA:HB2	1:51:A:TRP:HZ2	19	0.2
(1,1240)	1:4:A:ALA:HB3	1:51:A:TRP:HZ2	19	0.2
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	17	0.2
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	7	0.2
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	7	0.2
(1,1129)	1:122:A:ARG:H	1:122:A:ARG:HB3	8	0.2
(1,1123)	1:25:A:GLY:H	1:45:A:CYS:HA	6	0.2
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	14	0.2
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	14	0.2
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	14	0.2
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG11	17	0.2
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG12	17	0.2
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG13	17	0.2
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	5	0.2
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	5	0.2
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	5	0.2
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	11	0.2
(1,952)	1:107:A:SER:H	1:110:A:THR:H	20	0.2
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	19	0.2
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	2	0.2
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	9	0.2
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	9	0.2
(1,905)	1:1:A:GLN:HB2	1:1:A:GLN:HE22	10	0.2
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	19	0.2
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	6	0.2
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	6	0.2
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	14	0.2
(1,790)	1:16:A:LEU:H	1:28:A:LEU:HG	8	0.2
(1,786)	1:15:A:GLN:HB2	1:16:A:LEU:H	18	0.2
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	3	0.2
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	3	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	5	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	5	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	5	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	19	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	19	0.2
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	19	0.2
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	5	0.2
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	8	0.2
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	6	0.2
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	18	0.2
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	3	0.2
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	3	0.2
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	4	0.2
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	4	0.2
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	5	0.2
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	6	0.2
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	14	0.2
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	14	0.2
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	14	0.2
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	9	0.2
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	3	0.2
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	15	0.2
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	19	0.2
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	8	0.2
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	11	0.2
(1,418)	1:56:A:ASP:H	1:57:A:ARG:H	18	0.2
(1,415)	1:55:A:LYS:HA	1:57:A:ARG:H	18	0.2
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	3	0.2
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	20	0.2
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	15	0.2
(1,360)	1:105:A:ILE:H	1:114:A:ASP:HA	11	0.2
(1,290)	1:86:A:ILE:HD11	1:104:A:CYS:H	20	0.2
(1,290)	1:86:A:ILE:HD12	1:104:A:CYS:H	20	0.2
(1,290)	1:86:A:ILE:HD13	1:104:A:CYS:H	20	0.2
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	11	0.2
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	11	0.2
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	11	0.2
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	12	0.2
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	12	0.2
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	1	0.2
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	5	0.2
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	7	0.2
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	2	0.2
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	18	0.2
(1,83)	1:36:A:TYR:HE1	1:60:A:ARG:H	12	0.2
(1,83)	1:36:A:TYR:HE2	1:60:A:ARG:H	12	0.2
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	9	0.2
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	6	0.2
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	18	0.2
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	8	0.2
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	8	0.2
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	8	0.2
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	11	0.2
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	11	0.2
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	6	0.19
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	6	0.19
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	6	0.19
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	6	0.19
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	1	0.19
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	1	0.19
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	1	0.19
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	1	0.19
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	1	0.19
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	1	0.19
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	17	0.19
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	17	0.19
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	11	0.19
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	11	0.19
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	11	0.19
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	11	0.19
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	18	0.19
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	18	0.19
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	18	0.19
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	18	0.19
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB2	16	0.19
(1,2482)	1:94:A:TYR:HB3	1:122:A:ARG:HB3	16	0.19
(1,2461)	1:90:A:CYS:HB2	1:91:A:THR:H	17	0.19
(1,2461)	1:90:A:CYS:HB3	1:91:A:THR:H	17	0.19
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	7	0.19
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	7	0.19
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB2	5	0.19
(1,2436)	1:85:A:GLN:HG3	1:101:A:SER:HB3	5	0.19
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	9	0.19
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	9	0.19
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	9	0.19
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	9	0.19
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE1	19	0.19
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE2	19	0.19
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE3	19	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE1	19	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE2	19	0.19
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE3	19	0.19
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB2	2	0.19
(1,2321)	1:67:A:PRO:HG2	1:68:A:ASP:HB3	2	0.19
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	13	0.19
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	18	0.19
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	18	0.19
(1,2273)	1:61:A:LYS:HD2	1:111:A:VAL:H	11	0.19
(1,2273)	1:61:A:LYS:HD3	1:111:A:VAL:H	11	0.19
(1,2251)	1:60:A:ARG:HD2	1:82:A:PHE:H	17	0.19
(1,2251)	1:60:A:ARG:HD3	1:82:A:PHE:H	17	0.19
(1,2240)	1:60:A:ARG:HG2	1:61:A:LYS:H	17	0.19
(1,2240)	1:60:A:ARG:HG3	1:61:A:LYS:H	17	0.19
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	8	0.19
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	8	0.19
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	20	0.19
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	20	0.19
(1,2211)	1:55:A:LYS:HE2	1:56:A:ASP:H	20	0.19
(1,2211)	1:55:A:LYS:HE3	1:56:A:ASP:H	20	0.19
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	11	0.19
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	11	0.19
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	11	0.19
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	11	0.19
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	6	0.19
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	6	0.19
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG2	7	0.19
(1,2120)	1:37:A:SER:HB2	1:59:A:ARG:HG3	7	0.19
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG2	7	0.19
(1,2120)	1:37:A:SER:HB3	1:59:A:ARG:HG3	7	0.19
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	16	0.19
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	16	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	4	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	4	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	4	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD21	4	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD22	4	0.19
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD23	4	0.19
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	7	0.19
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	7	0.19
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	9	0.19
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	9	0.19
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	4	0.19
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	4	0.19
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	9	0.19
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	9	0.19
(1,1966)	1:34:A:PRO:HA	1:36:A:TYR:HD1	4	0.19
(1,1966)	1:34:A:PRO:HA	1:36:A:TYR:HD2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	6	0.19
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	6	0.19
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	6	0.19
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	6	0.19
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	6	0.19
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	6	0.19
(1,1889)	1:22:A:PHE:HB3	1:26:A:THR:HA	10	0.19
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	3	0.19
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	19	0.19
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	19	0.19
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	19	0.19
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	20	0.19
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	20	0.19
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	20	0.19
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE1	6	0.19
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE2	6	0.19
(1,1811)	1:71:A:ASN:HB2	1:73:A:MET:HE3	6	0.19
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	7	0.19
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	7	0.19
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	7	0.19
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	17	0.19
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	17	0.19
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	17	0.19
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD11	18	0.19
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD12	18	0.19
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD13	18	0.19
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD11	18	0.19
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD12	18	0.19
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD13	18	0.19
(1,1750)	1:8:A:LEU:HG	1:10:A:PHE:HB3	17	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	5	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	5	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	5	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	13	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	13	0.19
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	13	0.19
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	17	0.19
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	17	0.19
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	11	0.19
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	20	0.19
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	20	0.19
(1,1574)	1:87:A:LYS:HA	1:100:A:SER:HA	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	14	0.19
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	14	0.19
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	14	0.19
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	10	0.19
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	10	0.19
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	10	0.19
(1,1452)	1:2:A:CYS:HB2	1:5:A:PRO:HA	12	0.19
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	13	0.19
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	13	0.19
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	13	0.19
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG21	5	0.19
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG22	5	0.19
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG23	5	0.19
(1,1242)	1:3:A:ASN:H	1:51:A:TRP:HZ2	16	0.19
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	4	0.19
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG21	14	0.19
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG22	14	0.19
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG23	14	0.19
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	12	0.19
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	12	0.19
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	12	0.19
(1,1044)	1:2:A:CYS:HB2	1:51:A:TRP:HD1	3	0.19
(1,1038)	1:57:A:ARG:HA	1:57:A:ARG:HD3	19	0.19
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	8	0.19
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	8	0.19
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	8	0.19
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	8	0.19
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	8	0.19
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	8	0.19
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	8	0.19
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	8	0.19
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	8	0.19
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD11	10	0.19
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD12	10	0.19
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD13	10	0.19
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD11	2	0.19
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD12	2	0.19
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD13	2	0.19
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	16	0.19
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	16	0.19
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	16	0.19
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	12	0.19
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	1	0.19
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	1	0.19
(1,914)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	17	0.19
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	8	0.19
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	17	0.19
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	13	0.19
(1,864)	1:27:A:TYR:HE1	1:42:A:SER:H	7	0.19
(1,864)	1:27:A:TYR:HE2	1:42:A:SER:H	7	0.19
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	18	0.19
(1,844)	1:28:A:LEU:HD11	1:29:A:ASN:H	14	0.19
(1,844)	1:28:A:LEU:HD12	1:29:A:ASN:H	14	0.19
(1,844)	1:28:A:LEU:HD13	1:29:A:ASN:H	14	0.19
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	2	0.19
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	4	0.19
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	6	0.19
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	9	0.19
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	9	0.19
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	12	0.19
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	12	0.19
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	14	0.19
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE1	13	0.19
(1,800)	1:19:A:GLU:H	1:20:A:PHE:HE2	13	0.19
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	20	0.19
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	20	0.19
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	12	0.19
(1,757)	1:24:A:ILE:HG13	1:49:A:SER:H	6	0.19
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	10	0.19
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	10	0.19
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	10	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	1	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	1	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	1	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	6	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	6	0.19
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	6	0.19
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	10	0.19
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	8	0.19
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	8	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	7	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	7	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	13	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	13	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	13	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	16	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	16	0.19
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	16	0.19
(1,583)	1:26:A:THR:H	1:51:A:TRP:HH2	16	0.19
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	11	0.19
(1,569)	1:74:A:VAL:HG11	1:87:A:LYS:H	4	0.19
(1,569)	1:74:A:VAL:HG12	1:87:A:LYS:H	4	0.19
(1,569)	1:74:A:VAL:HG13	1:87:A:LYS:H	4	0.19
(1,537)	1:90:A:CYS:HB2	1:91:A:THR:H	14	0.19
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	1	0.19
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	16	0.19
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	18	0.19
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	19	0.19
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	17	0.19
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	19	0.19
(1,270)	1:33:A:ARG:H	1:36:A:TYR:HB2	14	0.19
(1,228)	1:111:A:VAL:HG21	1:113:A:TRP:H	17	0.19
(1,228)	1:111:A:VAL:HG22	1:113:A:TRP:H	17	0.19
(1,228)	1:111:A:VAL:HG23	1:113:A:TRP:H	17	0.19
(1,150)	1:92:A:LYS:HB2	1:93:A:GLY:H	6	0.19
(1,148)	1:74:A:VAL:HG11	1:89:A:SER:H	4	0.19
(1,148)	1:74:A:VAL:HG12	1:89:A:SER:H	4	0.19
(1,148)	1:74:A:VAL:HG13	1:89:A:SER:H	4	0.19
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	9	0.19
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	16	0.19
(1,120)	1:69:A:PRO:HB2	1:72:A:GLY:H	9	0.19
(1,120)	1:69:A:PRO:HB2	1:72:A:GLY:H	19	0.19
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE1	6	0.19
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE2	6	0.19
(1,117)	1:72:A:GLY:H	1:73:A:MET:HE3	6	0.19
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	8	0.19
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	8	0.19
(1,81)	1:60:A:ARG:H	1:60:A:ARG:HD3	2	0.19
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	8	0.19
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	10	0.19
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	12	0.19
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	17	0.19
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	18	0.19
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:36:A:TYR:HE1	1:37:A:SER:H	8	0.19
(1,23)	1:36:A:TYR:HE2	1:37:A:SER:H	8	0.19
(1,14)	1:95:A:ARG:H	1:121:A:ASP:HA	12	0.19
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	14	0.18
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	14	0.18
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	12	0.18
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	12	0.18
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	12	0.18
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	12	0.18
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	14	0.18
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	14	0.18
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	13	0.18
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	13	0.18
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	11	0.18
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	11	0.18
(1,2363)	1:73:A:MET:HG2	1:90:A:CYS:HA	8	0.18
(1,2363)	1:73:A:MET:HG3	1:90:A:CYS:HA	8	0.18
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB2	12	0.18
(1,2361)	1:73:A:MET:HB2	1:89:A:SER:HB3	12	0.18
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB2	12	0.18
(1,2361)	1:73:A:MET:HB3	1:89:A:SER:HB3	12	0.18
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	17	0.18
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	17	0.18
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	3	0.18
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	3	0.18
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	19	0.18
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	19	0.18
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	15	0.18
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	15	0.18
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	10	0.18
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	10	0.18
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	2	0.18
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	2	0.18
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	4	0.18
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	4	0.18
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	4	0.18
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	4	0.18
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	12	0.18
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	12	0.18
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	12	0.18
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	12	0.18
(1,2246)	1:60:A:ARG:HG2	1:82:A:PHE:HD1	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2246)	1:60:A:ARG:HG2	1:82:A:PHE:HD2	16	0.18
(1,2246)	1:60:A:ARG:HG3	1:82:A:PHE:HD1	16	0.18
(1,2246)	1:60:A:ARG:HG3	1:82:A:PHE:HD2	16	0.18
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	4	0.18
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	4	0.18
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	19	0.18
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	19	0.18
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	19	0.18
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	19	0.18
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	4	0.18
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	4	0.18
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	20	0.18
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	20	0.18
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	18	0.18
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	18	0.18
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	18	0.18
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	18	0.18
(1,2169)	1:47:A:LYS:HE2	1:48:A:ASN:H	18	0.18
(1,2169)	1:47:A:LYS:HE3	1:48:A:ASN:H	18	0.18
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	14	0.18
(1,2159)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	14	0.18
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	14	0.18
(1,2159)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	14	0.18
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	8	0.18
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	8	0.18
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	8	0.18
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	8	0.18
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	8	0.18
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	8	0.18
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA2	7	0.18
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA3	7	0.18
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA2	7	0.18
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA3	7	0.18
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA2	7	0.18
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA3	7	0.18
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	10	0.18
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	10	0.18
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	10	0.18
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	10	0.18
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	13	0.18
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	13	0.18
(1,2101)	1:31:A:GLU:HB2	1:32:A:CYS:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2101)	1:31:A:GLU:HB3	1:32:A:CYS:H	3	0.18
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG2	7	0.18
(1,2073)	1:21:A:GLU:H	1:21:A:GLU:HG3	7	0.18
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	15	0.18
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	15	0.18
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	15	0.18
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	15	0.18
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	15	0.18
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	15	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	13	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	13	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	13	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	13	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	13	0.18
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD11	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD12	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD13	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD21	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD22	13	0.18
(1,2044)	1:15:A:GLN:H	1:16:A:LEU:HD23	13	0.18
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	16	0.18
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	16	0.18
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	5	0.18
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	5	0.18
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	3	0.18
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	7	0.18
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	16	0.18
(1,1895)	1:15:A:GLN:HE22	1:28:A:LEU:HD21	2	0.18
(1,1895)	1:15:A:GLN:HE22	1:28:A:LEU:HD22	2	0.18
(1,1895)	1:15:A:GLN:HE22	1:28:A:LEU:HD23	2	0.18
(1,1889)	1:22:A:PHE:HB3	1:26:A:THR:HA	20	0.18
(1,1875)	1:45:A:CYS:HA	1:50:A:VAL:HB	10	0.18
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	16	0.18
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	16	0.18
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	16	0.18
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	16	0.18
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	16	0.18
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	16	0.18
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	5	0.18
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	5	0.18
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG2	19	0.18
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG3	19	0.18
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	15	0.18
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	15	0.18
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	15	0.18
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD11	1	0.18
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD12	1	0.18
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD13	1	0.18
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD11	1	0.18
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD12	1	0.18
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD13	1	0.18
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	13	0.18
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	13	0.18
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	13	0.18
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	15	0.18
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	15	0.18
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	15	0.18
(1,1696)	1:22:A:PHE:HD1	1:26:A:THR:HB	10	0.18
(1,1696)	1:22:A:PHE:HD2	1:26:A:THR:HB	10	0.18
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	9	0.18
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	12	0.18
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	16	0.18
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	2	0.18
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	2	0.18
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	18	0.18
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	18	0.18
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	18	0.18
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	18	0.18
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	18	0.18
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	18	0.18
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	12	0.18
(1,1542)	1:47:A:LYS:HA	1:47:A:LYS:HE2	17	0.18
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	14	0.18
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	14	0.18
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	14	0.18
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	14	0.18
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	14	0.18
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	14	0.18
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	4	0.18
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	4	0.18
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	4	0.18
(1,1476)	1:78:A:LYS:HB2	1:80:A:ILE:HA	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:96:A:LEU:HG	1:119:A:ILE:H	7	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	4	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	4	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	4	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	19	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	19	0.18
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	19	0.18
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	20	0.18
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	20	0.18
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	20	0.18
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	10	0.18
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	10	0.18
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	2	0.18
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	2	0.18
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	2	0.18
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	9	0.18
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	9	0.18
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	9	0.18
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	13	0.18
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	13	0.18
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	13	0.18
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	10	0.18
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	20	0.18
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD1	8	0.18
(1,1147)	1:60:A:ARG:HA	1:82:A:PHE:HD2	8	0.18
(1,1139)	1:57:A:ARG:HA	1:57:A:ARG:HD2	2	0.18
(1,1096)	1:17:A:THR:HG21	1:19:A:GLU:HG3	13	0.18
(1,1096)	1:17:A:THR:HG22	1:19:A:GLU:HG3	13	0.18
(1,1096)	1:17:A:THR:HG23	1:19:A:GLU:HG3	13	0.18
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	11	0.18
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	11	0.18
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	6	0.18
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	6	0.18
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	6	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD11	12	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD12	12	0.18
(1,1012)	1:60:A:ARG:HB3	1:106:A:ILE:HD13	12	0.18
(1,1006)	1:43:A:ILE:HG21	1:51:A:TRP:HD1	8	0.18
(1,1006)	1:43:A:ILE:HG22	1:51:A:TRP:HD1	8	0.18
(1,1006)	1:43:A:ILE:HG23	1:51:A:TRP:HD1	8	0.18
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	6	0.18
(1,979)	1:60:A:ARG:HB3	1:106:A:ILE:HG13	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:60:A:ARG:HB2	1:106:A:ILE:HG13	8	0.18
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	4	0.18
(1,927)	1:65:A:ASN:HD21	1:68:A:ASP:HA	14	0.18
(1,893)	1:3:A:ASN:HA	1:3:A:ASN:HD21	12	0.18
(1,887)	1:4:A:ALA:HB1	1:51:A:TRP:HE1	19	0.18
(1,887)	1:4:A:ALA:HB2	1:51:A:TRP:HE1	19	0.18
(1,887)	1:4:A:ALA:HB3	1:51:A:TRP:HE1	19	0.18
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	14	0.18
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	11	0.18
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	11	0.18
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	4	0.18
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	14	0.18
(1,864)	1:27:A:TYR:HE1	1:42:A:SER:H	5	0.18
(1,864)	1:27:A:TYR:HE2	1:42:A:SER:H	5	0.18
(1,862)	1:13:A:PRO:HA	1:31:A:GLU:H	1	0.18
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	7	0.18
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	19	0.18
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	17	0.18
(1,801)	1:16:A:LEU:HA	1:19:A:GLU:H	20	0.18
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	7	0.18
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	9	0.18
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	9	0.18
(1,757)	1:24:A:ILE:HG13	1:49:A:SER:H	11	0.18
(1,748)	1:24:A:ILE:H	1:24:A:ILE:HD11	5	0.18
(1,748)	1:24:A:ILE:H	1:24:A:ILE:HD12	5	0.18
(1,748)	1:24:A:ILE:H	1:24:A:ILE:HD13	5	0.18
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	12	0.18
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	12	0.18
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	12	0.18
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD1	1	0.18
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD2	1	0.18
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	2	0.18
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	3	0.18
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	7	0.18
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	8	0.18
(1,639)	1:45:A:CYS:H	1:51:A:TRP:HB3	2	0.18
(1,628)	1:77:A:ILE:H	1:86:A:ILE:HB	13	0.18
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	16	0.18
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	10	0.18
(1,520)	1:95:A:ARG:H	1:96:A:LEU:H	13	0.18
(1,486)	1:96:A:LEU:HB3	1:100:A:SER:H	4	0.18
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	3	0.18
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	7	0.18
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	11	0.18
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	10	0.18
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	15	0.18
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	15	0.18
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	3	0.18
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	3	0.18
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	10	0.18
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	10	0.18
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	15	0.18
(1,88)	1:96:A:LEU:HD11	1:97:A:ILE:H	1	0.18
(1,88)	1:96:A:LEU:HD12	1:97:A:ILE:H	1	0.18
(1,88)	1:96:A:LEU:HD13	1:97:A:ILE:H	1	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	1	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	1	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	13	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	13	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	15	0.18
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	15	0.18
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	4	0.18
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	8	0.18
(1,23)	1:36:A:TYR:HE1	1:37:A:SER:H	7	0.18
(1,23)	1:36:A:TYR:HE2	1:37:A:SER:H	7	0.18
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	10	0.18
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	10	0.18
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	10	0.18
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	2	0.17
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	2	0.17
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	1	0.17
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	1	0.17
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	1	0.17
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	1	0.17
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	1	0.17
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	1	0.17
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	3	0.17
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	3	0.17
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	3	0.17
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	3	0.17
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	14	0.17
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	14	0.17
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	3	0.17
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	3	0.17
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	3	0.17
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	16	0.17
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	16	0.17
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	16	0.17
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	16	0.17
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	16	0.17
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	16	0.17
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG2	12	0.17
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG3	12	0.17
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	9	0.17
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	9	0.17
(1,2319)	1:67:A:PRO:HA	1:68:A:ASP:HB2	7	0.17
(1,2319)	1:67:A:PRO:HA	1:68:A:ASP:HB3	7	0.17
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	2	0.17
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	2	0.17
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	4	0.17
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	4	0.17
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	1	0.17
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	1	0.17
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG11	7	0.17
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG12	7	0.17
(1,2247)	1:60:A:ARG:HG2	1:111:A:VAL:HG13	7	0.17
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG11	7	0.17
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG12	7	0.17
(1,2247)	1:60:A:ARG:HG3	1:111:A:VAL:HG13	7	0.17
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	7	0.17
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	7	0.17
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	18	0.17
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	18	0.17
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	3	0.17
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	3	0.17
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	17	0.17
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	17	0.17
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	5	0.17
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	5	0.17
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	18	0.17
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	18	0.17
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	18	0.17
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	18	0.17
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	18	0.17
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	3	0.17
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	3	0.17
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	2	0.17
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	2	0.17
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	19	0.17
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	19	0.17
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD11	19	0.17
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD12	19	0.17
(1,2109)	1:35:A:GLY:HA2	1:106:A:ILE:HD13	19	0.17
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD11	19	0.17
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD12	19	0.17
(1,2109)	1:35:A:GLY:HA3	1:106:A:ILE:HD13	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	19	0.17
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	19	0.17
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	19	0.17
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB2	4	0.17
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB3	4	0.17
(1,2056)	1:16:A:LEU:HD11	1:17:A:THR:HB	20	0.17
(1,2056)	1:16:A:LEU:HD12	1:17:A:THR:HB	20	0.17
(1,2056)	1:16:A:LEU:HD13	1:17:A:THR:HB	20	0.17
(1,2056)	1:16:A:LEU:HD21	1:17:A:THR:HB	20	0.17
(1,2056)	1:16:A:LEU:HD22	1:17:A:THR:HB	20	0.17
(1,2056)	1:16:A:LEU:HD23	1:17:A:THR:HB	20	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	1	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	9	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	9	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	9	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	9	0.17
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	9	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	1	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	1	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	5	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	5	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB2	12	0.17
(1,1984)	1:3:A:ASN:H	1:3:A:ASN:HB3	12	0.17
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	1	0.17
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	1	0.17
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	3	0.17
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	3	0.17
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	17	0.17
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	17	0.17
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	17	0.17
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	17	0.17
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	17	0.17
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	17	0.17
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	8	0.17
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	8	0.17
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	9	0.17
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	4	0.17
(1,1889)	1:22:A:PHE:HB3	1:26:A:THR:HA	19	0.17
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	4	0.17
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	8	0.17
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	13	0.17
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	20	0.17
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG2	14	0.17
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG3	14	0.17
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	8	0.17
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	8	0.17
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	8	0.17
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	18	0.17
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	18	0.17
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	18	0.17
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	13	0.17
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	13	0.17
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	15	0.17
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	15	0.17
(1,1685)	1:85:A:GLN:HB3	1:103:A:THR:HA	18	0.17
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	18	0.17
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	18	0.17
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	5	0.17
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	2	0.17
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	2	0.17
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	2	0.17
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	7	0.17
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	7	0.17
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	7	0.17
(1,1574)	1:87:A:LYS:HA	1:100:A:SER:HA	13	0.17
(1,1560)	1:5:A:PRO:HB2	1:6:A:GLU:HA	3	0.17
(1,1560)	1:5:A:PRO:HB2	1:6:A:GLU:HA	5	0.17
(1,1550)	1:97:A:ILE:HD11	1:121:A:ASP:HA	2	0.17
(1,1550)	1:97:A:ILE:HD12	1:121:A:ASP:HA	2	0.17
(1,1550)	1:97:A:ILE:HD13	1:121:A:ASP:HA	2	0.17
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD11	12	0.17
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD12	12	0.17
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD13	12	0.17
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	15	0.17
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	15	0.17
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	15	0.17
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	15	0.17
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	15	0.17
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	15	0.17
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	2	0.17
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	2	0.17
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	2	0.17
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	15	0.17
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	15	0.17
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	15	0.17
(1,1461)	1:4:A:ALA:H	1:20:A:PHE:HA	16	0.17
(1,1458)	1:61:A:LYS:HB3	1:62:A:SER:HA	4	0.17
(1,1439)	1:44:A:ILE:HD11	1:51:A:TRP:HA	10	0.17
(1,1439)	1:44:A:ILE:HD12	1:51:A:TRP:HA	10	0.17
(1,1439)	1:44:A:ILE:HD13	1:51:A:TRP:HA	10	0.17
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	9	0.17
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	9	0.17
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	9	0.17
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	4	0.17
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	16	0.17
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	16	0.17
(1,1308)	1:67:A:PRO:HG2	1:68:A:ASP:HA	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	3	0.17
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	16	0.17
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	16	0.17
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	16	0.17
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	6	0.17
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	6	0.17
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	18	0.17
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	18	0.17
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	18	0.17
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG21	17	0.17
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG22	17	0.17
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG23	17	0.17
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	3	0.17
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	8	0.17
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	15	0.17
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	14	0.17
(1,1156)	1:73:A:MET:HB2	1:89:A:SER:H	12	0.17
(1,1156)	1:73:A:MET:HB3	1:89:A:SER:H	12	0.17
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	1	0.17
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	1	0.17
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	11	0.17
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	11	0.17
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB2	12	0.17
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB3	12	0.17
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	6	0.17
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	6	0.17
(1,1067)	1:110:A:THR:HB	1:112:A:ILE:HG21	7	0.17
(1,1067)	1:110:A:THR:HB	1:112:A:ILE:HG22	7	0.17
(1,1067)	1:110:A:THR:HB	1:112:A:ILE:HG23	7	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	2	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	2	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	2	0.17
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	2	0.17
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	2	0.17
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	2	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	2	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	2	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	2	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	6	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	6	0.17
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	6	0.17
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	6	0.17
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	6	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	6	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	6	0.17
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	6	0.17
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG21	19	0.17
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG22	19	0.17
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG23	19	0.17
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG21	8	0.17
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG22	8	0.17
(1,997)	1:81:A:GLN:HE21	1:111:A:VAL:HG23	8	0.17
(1,954)	1:68:A:ASP:H	1:69:A:PRO:HA	16	0.17
(1,952)	1:107:A:SER:H	1:110:A:THR:H	11	0.17
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	2	0.17
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	7	0.17
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	19	0.17
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	19	0.17
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	19	0.17
(1,917)	1:13:A:PRO:HG2	1:15:A:GLN:HE22	11	0.17
(1,917)	1:13:A:PRO:HG3	1:15:A:GLN:HE22	11	0.17
(1,915)	1:15:A:GLN:HB3	1:15:A:GLN:HE21	18	0.17
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	5	0.17
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	19	0.17
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	9	0.17
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	19	0.17
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	7	0.17
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	9	0.17
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	1	0.17
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	13	0.17
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	18	0.17
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	6	0.17
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	2	0.17
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	13	0.17
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	13	0.17
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	9	0.17
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	14	0.17
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	14	0.17
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	20	0.17
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	3	0.17
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	3	0.17
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	3	0.17
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	11	0.17
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	2	0.17
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	2	0.17
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	2	0.17
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	10	0.17
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	15	0.17
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	19	0.17
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	4	0.17
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	8	0.17
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	17	0.17
(1,523)	1:90:A:CYS:H	1:96:A:LEU:H	14	0.17
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	18	0.17
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	18	0.17
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	17	0.17
(1,447)	1:106:A:ILE:HG21	1:108:A:GLY:H	7	0.17
(1,447)	1:106:A:ILE:HG22	1:108:A:GLY:H	7	0.17
(1,447)	1:106:A:ILE:HG23	1:108:A:GLY:H	7	0.17
(1,425)	1:102:A:ALA:HB1	1:116:A:GLU:H	19	0.17
(1,425)	1:102:A:ALA:HB2	1:116:A:GLU:H	19	0.17
(1,425)	1:102:A:ALA:HB3	1:116:A:GLU:H	19	0.17
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	2	0.17
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	8	0.17
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	12	0.17
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	14	0.17
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	14	0.17
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	9	0.17
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	9	0.17
(1,156)	1:93:A:GLY:H	1:94:A:TYR:H	13	0.17
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	16	0.17
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	3	0.17
(1,48)	1:12:A:ARG:H	1:32:A:CYS:H	6	0.17
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	12	0.17
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	14	0.17
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	14	0.17
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	14	0.17
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	14	0.17
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	16	0.17
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	16	0.17
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	16	0.17
(1,2550)	1:105:A:ILE:H	1:114:A:ASP:HB2	17	0.16
(1,2550)	1:105:A:ILE:H	1:114:A:ASP:HB3	17	0.16
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	9	0.16
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	9	0.16
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	9	0.16
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD11	1:119:A:ILE:HD13	17	0.16
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD12	1:119:A:ILE:HD13	17	0.16
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD13	1:119:A:ILE:HD13	17	0.16
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD21	1:119:A:ILE:HD13	17	0.16
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD22	1:119:A:ILE:HD13	17	0.16
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD11	17	0.16
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD12	17	0.16
(1,2514)	1:96:A:LEU:HD23	1:119:A:ILE:HD13	17	0.16
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	3	0.16
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	3	0.16
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	19	0.16
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	19	0.16
(1,2477)	1:92:A:LYS:HG2	1:93:A:GLY:HA2	15	0.16
(1,2477)	1:92:A:LYS:HG3	1:93:A:GLY:HA2	15	0.16
(1,2461)	1:90:A:CYS:HB2	1:91:A:THR:H	9	0.16
(1,2461)	1:90:A:CYS:HB3	1:91:A:THR:H	9	0.16
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	17	0.16
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	17	0.16
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	2	0.16
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	2	0.16
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	7	0.16
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	7	0.16
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	3	0.16
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	3	0.16
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	16	0.16
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	16	0.16
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	13	0.16
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	13	0.16
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	14	0.16
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	14	0.16
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	14	0.16
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	14	0.16
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	14	0.16
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG2	9	0.16
(1,2357)	1:73:A:MET:H	1:73:A:MET:HG3	9	0.16
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA2	16	0.16
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA3	16	0.16
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	10	0.16
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	10	0.16
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	19	0.16
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	19	0.16
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	19	0.16
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	19	0.16
(1,2289)	1:63:A:CYS:HB2	1:81:A:GLN:H	1	0.16
(1,2289)	1:63:A:CYS:HB3	1:81:A:GLN:H	1	0.16
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	10	0.16
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	10	0.16
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	10	0.16
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	10	0.16
(1,2213)	1:55:A:LYS:HE2	1:57:A:ARG:H	12	0.16
(1,2213)	1:55:A:LYS:HE3	1:57:A:ARG:H	12	0.16
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	18	0.16
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	18	0.16
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE2	16	0.16
(1,2200)	1:55:A:LYS:HA	1:55:A:LYS:HE3	16	0.16
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB2	12	0.16
(1,2173)	1:48:A:ASN:HB2	1:49:A:SER:HB3	12	0.16
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB2	12	0.16
(1,2173)	1:48:A:ASN:HB3	1:49:A:SER:HB3	12	0.16
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	2	0.16
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	2	0.16
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	2	0.16
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	2	0.16
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	2	0.16
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	2	0.16
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB2	2	0.16
(1,2125)	1:39:A:ARG:H	1:39:A:ARG:HB3	2	0.16
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	6	0.16
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	6	0.16
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	4	0.16
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	4	0.16
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	4	0.16
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	4	0.16
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	4	0.16
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	16	0.16
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	16	0.16
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	16	0.16
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	16	0.16
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	16	0.16
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	16	0.16
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	20	0.16
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	20	0.16
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	20	0.16
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	20	0.16
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	20	0.16
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	20	0.16
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB2	13	0.16
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB3	13	0.16
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD3	16	0.16
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD3	16	0.16
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD3	16	0.16
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD3	16	0.16
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD3	16	0.16
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD2	16	0.16
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD3	16	0.16
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG2	11	0.16
(1,1997)	1:6:A:GLU:H	1:6:A:GLU:HG3	11	0.16
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	6	0.16
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	6	0.16
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	7	0.16
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	7	0.16
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	11	0.16
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	11	0.16
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	17	0.16
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	13	0.16
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1898)	1:15:A:GLN:HB3	1:15:A:GLN:HE22	18	0.16
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	6	0.16
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	6	0.16
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	6	0.16
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	6	0.16
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	6	0.16
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	6	0.16
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	6	0.16
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	11	0.16
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	11	0.16
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	11	0.16
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	11	0.16
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	11	0.16
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	11	0.16
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	16	0.16
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	16	0.16
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	15	0.16
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	16	0.16
(1,1832)	1:80:A:ILE:HA	1:80:A:ILE:HD11	2	0.16
(1,1832)	1:80:A:ILE:HA	1:80:A:ILE:HD12	2	0.16
(1,1832)	1:80:A:ILE:HA	1:80:A:ILE:HD13	2	0.16
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG2	5	0.16
(1,1816)	1:22:A:PHE:HB3	1:23:A:PRO:HG3	5	0.16
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	9	0.16
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	9	0.16
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	9	0.16
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD11	16	0.16
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD12	16	0.16
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD13	16	0.16
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD11	16	0.16
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD12	16	0.16
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD13	16	0.16
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	19	0.16
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	19	0.16
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	19	0.16
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	16	0.16
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	16	0.16
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	7	0.16
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	5	0.16
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	5	0.16
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	5	0.16
(1,1719)	1:43:A:ILE:HD11	1:54:A:ALA:HB1	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:43:A:ILE:HD11	1:54:A:ALA:HB2	20	0.16
(1,1719)	1:43:A:ILE:HD11	1:54:A:ALA:HB3	20	0.16
(1,1719)	1:43:A:ILE:HD12	1:54:A:ALA:HB1	20	0.16
(1,1719)	1:43:A:ILE:HD12	1:54:A:ALA:HB2	20	0.16
(1,1719)	1:43:A:ILE:HD12	1:54:A:ALA:HB3	20	0.16
(1,1719)	1:43:A:ILE:HD13	1:54:A:ALA:HB1	20	0.16
(1,1719)	1:43:A:ILE:HD13	1:54:A:ALA:HB2	20	0.16
(1,1719)	1:43:A:ILE:HD13	1:54:A:ALA:HB3	20	0.16
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	9	0.16
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	9	0.16
(1,1692)	1:97:A:ILE:HG12	1:121:A:ASP:HA	15	0.16
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	3	0.16
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	18	0.16
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	20	0.16
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	10	0.16
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	10	0.16
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	10	0.16
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	10	0.16
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	10	0.16
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	10	0.16
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD1	19	0.16
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD2	19	0.16
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	6	0.16
(1,1629)	1:87:A:LYS:HA	1:87:A:LYS:HG3	10	0.16
(1,1580)	1:4:A:ALA:HB1	1:20:A:PHE:HA	1	0.16
(1,1580)	1:4:A:ALA:HB2	1:20:A:PHE:HA	1	0.16
(1,1580)	1:4:A:ALA:HB3	1:20:A:PHE:HA	1	0.16
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	3	0.16
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	3	0.16
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	6	0.16
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	6	0.16
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	6	0.16
(1,1532)	1:105:A:ILE:HD11	1:114:A:ASP:HB2	1	0.16
(1,1532)	1:105:A:ILE:HD12	1:114:A:ASP:HB2	1	0.16
(1,1532)	1:105:A:ILE:HD13	1:114:A:ASP:HB2	1	0.16
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	14	0.16
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	14	0.16
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	14	0.16
(1,1504)	1:73:A:MET:HE1	1:91:A:THR:HB	6	0.16
(1,1504)	1:73:A:MET:HE2	1:91:A:THR:HB	6	0.16
(1,1504)	1:73:A:MET:HE3	1:91:A:THR:HB	6	0.16
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	1	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	1	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	1	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	15	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	15	0.16
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	15	0.16
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	7	0.16
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	7	0.16
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	7	0.16
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	1	0.16
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	1	0.16
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	1	0.16
(1,1242)	1:3:A:ASN:H	1:51:A:TRP:HZ2	8	0.16
(1,1237)	1:22:A:PHE:HB2	1:51:A:TRP:HZ2	5	0.16
(1,1231)	1:105:A:ILE:HG21	1:113:A:TRP:HE3	6	0.16
(1,1231)	1:105:A:ILE:HG22	1:113:A:TRP:HE3	6	0.16
(1,1231)	1:105:A:ILE:HG23	1:113:A:TRP:HE3	6	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	3	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	3	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	3	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	15	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	15	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	15	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	20	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	20	0.16
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	20	0.16
(1,1178)	1:84:A:SER:HA	1:103:A:THR:HG21	11	0.16
(1,1178)	1:84:A:SER:HA	1:103:A:THR:HG22	11	0.16
(1,1178)	1:84:A:SER:HA	1:103:A:THR:HG23	11	0.16
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	5	0.16
(1,1143)	1:10:A:PHE:HD1	1:57:A:ARG:HB3	18	0.16
(1,1143)	1:10:A:PHE:HD2	1:57:A:ARG:HB3	18	0.16
(1,1130)	1:122:A:ARG:H	1:122:A:ARG:HB2	17	0.16
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD11	14	0.16
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD12	14	0.16
(1,1124)	1:45:A:CYS:HA	1:46:A:LEU:HD13	14	0.16
(1,1075)	1:5:A:PRO:HB2	1:51:A:TRP:HD1	13	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	5	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	5	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	5	0.16
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	5	0.16
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	5	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	5	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	5	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	5	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	11	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	11	0.16
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	11	0.16
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	11	0.16
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	11	0.16
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	11	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	11	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	11	0.16
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	11	0.16
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	20	0.16
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	20	0.16
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	20	0.16
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD11	12	0.16
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD12	12	0.16
(1,1016)	1:43:A:ILE:HD11	1:44:A:ILE:HD13	12	0.16
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD11	12	0.16
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD12	12	0.16
(1,1016)	1:43:A:ILE:HD12	1:44:A:ILE:HD13	12	0.16
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD11	12	0.16
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD12	12	0.16
(1,1016)	1:43:A:ILE:HD13	1:44:A:ILE:HD13	12	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	4	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	4	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	4	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	19	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	19	0.16
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	19	0.16
(1,959)	1:22:A:PHE:H	1:51:A:TRP:HE1	19	0.16
(1,952)	1:107:A:SER:H	1:110:A:THR:H	13	0.16
(1,929)	1:65:A:ASN:HD22	1:68:A:ASP:HA	17	0.16
(1,926)	1:65:A:ASN:HA	1:65:A:ASN:HD21	4	0.16
(1,924)	1:15:A:GLN:HE22	1:28:A:LEU:HD11	4	0.16
(1,924)	1:15:A:GLN:HE22	1:28:A:LEU:HD12	4	0.16
(1,924)	1:15:A:GLN:HE22	1:28:A:LEU:HD13	4	0.16
(1,923)	1:15:A:GLN:HE21	1:28:A:LEU:HG	14	0.16
(1,898)	1:1:A:GLN:H	1:1:A:GLN:HE22	20	0.16
(1,893)	1:3:A:ASN:HA	1:3:A:ASN:HD21	1	0.16
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	12	0.16
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	16	0.16
(1,842)	1:29:A:ASN:H	1:29:A:ASN:HB3	20	0.16
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	10	0.16
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	16	0.16
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	7	0.16
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	16	0.16
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	9	0.16
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	9	0.16
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	6	0.16
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	6	0.16
(1,794)	1:16:A:LEU:HA	1:18:A:ASP:H	9	0.16
(1,790)	1:16:A:LEU:H	1:28:A:LEU:HG	11	0.16
(1,758)	1:46:A:LEU:H	1:50:A:VAL:H	7	0.16
(1,751)	1:47:A:LYS:HA	1:48:A:ASN:H	20	0.16
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	14	0.16
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	14	0.16
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	14	0.16
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	15	0.16
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	15	0.16
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	15	0.16
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	3	0.16
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	15	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	14	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	14	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	14	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	16	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	16	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	16	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	18	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	18	0.16
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	18	0.16
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	14	0.16
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	5	0.16
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	7	0.16
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD1	4	0.16
(1,662)	1:22:A:PHE:H	1:22:A:PHE:HD2	4	0.16
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	5	0.16
(1,622)	1:43:A:ILE:HG21	1:44:A:ILE:H	12	0.16
(1,622)	1:43:A:ILE:HG22	1:44:A:ILE:H	12	0.16
(1,622)	1:43:A:ILE:HG23	1:44:A:ILE:H	12	0.16
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:22:A:PHE:HB2	1:26:A:THR:H	20	0.16
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	19	0.16
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	17	0.16
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	10	0.16
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	1	0.16
(1,403)	1:99:A:SER:HB3	1:115:A:GLN:H	2	0.16
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	8	0.16
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	8	0.16
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	5	0.16
(1,261)	1:54:A:ALA:H	1:55:A:LYS:H	4	0.16
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	1	0.16
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	11	0.16
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	20	0.16
(1,187)	1:88:A:TYR:HB2	1:119:A:ILE:H	15	0.16
(1,187)	1:88:A:TYR:HB2	1:119:A:ILE:H	18	0.16
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	9	0.16
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	10	0.16
(1,183)	1:99:A:SER:H	1:119:A:ILE:H	2	0.16
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	8	0.16
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	7	0.16
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	7	0.16
(1,161)	1:14:A:THR:H	1:29:A:ASN:H	12	0.16
(1,161)	1:14:A:THR:H	1:29:A:ASN:H	15	0.16
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	6	0.16
(1,139)	1:80:A:ILE:H	1:81:A:GLN:H	17	0.16
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	6	0.16
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	1	0.16
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	15	0.16
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	7	0.16
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	13	0.16
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD11	9	0.16
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD12	9	0.16
(1,7)	1:95:A:ARG:H	1:97:A:ILE:HD13	9	0.16
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	12	0.15
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	12	0.15
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	12	0.15
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	12	0.15
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	12	0.15
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	12	0.15
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG11	13	0.15
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG12	13	0.15
(1,2555)	1:107:A:SER:HB2	1:111:A:VAL:HG13	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG11	13	0.15
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG12	13	0.15
(1,2555)	1:107:A:SER:HB3	1:111:A:VAL:HG13	13	0.15
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	17	0.15
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	17	0.15
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	17	0.15
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	17	0.15
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG2	17	0.15
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG3	17	0.15
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	3	0.15
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	3	0.15
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	3	0.15
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	3	0.15
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	3	0.15
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	3	0.15
(1,2507)	1:96:A:LEU:HD11	1:100:A:SER:HA	14	0.15
(1,2507)	1:96:A:LEU:HD12	1:100:A:SER:HA	14	0.15
(1,2507)	1:96:A:LEU:HD13	1:100:A:SER:HA	14	0.15
(1,2507)	1:96:A:LEU:HD21	1:100:A:SER:HA	14	0.15
(1,2507)	1:96:A:LEU:HD22	1:100:A:SER:HA	14	0.15
(1,2507)	1:96:A:LEU:HD23	1:100:A:SER:HA	14	0.15
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	1	0.15
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	1	0.15
(1,2443)	1:87:A:LYS:HB2	1:87:A:LYS:HE2	5	0.15
(1,2443)	1:87:A:LYS:HB2	1:87:A:LYS:HE3	5	0.15
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	13	0.15
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	13	0.15
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	14	0.15
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	14	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	1	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	1	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	11	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	11	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	12	0.15
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	12	0.15
(1,2433)	1:85:A:GLN:HG2	1:87:A:LYS:HD2	12	0.15
(1,2433)	1:85:A:GLN:HG2	1:87:A:LYS:HD3	12	0.15
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE2	10	0.15
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE3	10	0.15
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG13	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG11	1:76:A:VAL:HG23	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG13	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG12	1:76:A:VAL:HG23	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG13	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG13	1:76:A:VAL:HG23	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG13	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG21	1:76:A:VAL:HG23	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG13	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG22	1:76:A:VAL:HG23	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG11	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG12	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG13	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG21	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG22	1	0.15
(1,2372)	1:74:A:VAL:HG23	1:76:A:VAL:HG23	1	0.15
(1,2350)	1:71:A:ASN:HB2	1:72:A:GLY:H	17	0.15
(1,2350)	1:71:A:ASN:HB3	1:72:A:GLY:H	17	0.15
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	2	0.15
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	2	0.15
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	6	0.15
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	6	0.15
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	13	0.15
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	13	0.15
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2277)	1:61:A:LYS:HE2	1:62:A:SER:HB3	16	0.15
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB2	16	0.15
(1,2277)	1:61:A:LYS:HE3	1:62:A:SER:HB3	16	0.15
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	18	0.15
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	18	0.15
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	18	0.15
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	18	0.15
(1,2244)	1:60:A:ARG:HG2	1:82:A:PHE:HB2	8	0.15
(1,2244)	1:60:A:ARG:HG3	1:82:A:PHE:HB2	8	0.15
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	14	0.15
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	14	0.15
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	1	0.15
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	1	0.15
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	1	0.15
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	1	0.15
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	1	0.15
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	1	0.15
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	2	0.15
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	2	0.15
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	3	0.15
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	3	0.15
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	3	0.15
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	3	0.15
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	3	0.15
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	3	0.15
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	15	0.15
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	15	0.15
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	15	0.15
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	15	0.15
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	15	0.15
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	15	0.15
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	7	0.15
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	7	0.15
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	10	0.15
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	10	0.15
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	10	0.15
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	10	0.15
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	10	0.15
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	10	0.15
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	2	0.15
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	2	0.15
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	2	0.15
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	2	0.15
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	2	0.15
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD11	1:57:A:ARG:HG3	19	0.15
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD12	1:57:A:ARG:HG3	19	0.15
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD13	1:57:A:ARG:HG3	19	0.15
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD21	1:57:A:ARG:HG3	19	0.15
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD22	1:57:A:ARG:HG3	19	0.15
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG2	19	0.15
(1,2032)	1:8:A:LEU:HD23	1:57:A:ARG:HG3	19	0.15
(1,1981)	1:1:A:GLN:HE21	1:21:A:GLU:HB2	10	0.15
(1,1981)	1:1:A:GLN:HE21	1:21:A:GLU:HB3	10	0.15
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	12	0.15
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	12	0.15
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	20	0.15
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	20	0.15
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	2	0.15
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	2	0.15
(1,1959)	1:43:A:ILE:HB	1:51:A:TRP:HD1	13	0.15
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	2	0.15
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	2	0.15
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	2	0.15
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	2	0.15
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	2	0.15
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	2	0.15
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	3	0.15
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	12	0.15
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	13	0.15
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	14	0.15
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	17	0.15
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	6	0.15
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	6	0.15
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	6	0.15
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	6	0.15
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	6	0.15
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	6	0.15
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	6	0.15
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	6	0.15
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	18	0.15
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	17	0.15
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	2	0.15
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	2	0.15
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	2	0.15
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	12	0.15
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	12	0.15
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	12	0.15
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	19	0.15
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	19	0.15
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	19	0.15
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	12	0.15
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	12	0.15
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	12	0.15
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	12	0.15
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	12	0.15
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	12	0.15
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	8	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	2	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	2	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	2	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	7	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	7	0.15
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	7	0.15
(1,1643)	1:74:A:VAL:HA	1:75:A:HIS:HB2	3	0.15
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	7	0.15
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	11	0.15
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	11	0.15
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	14	0.15
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	14	0.15
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	14	0.15
(1,1541)	1:47:A:LYS:HA	1:47:A:LYS:HE3	5	0.15
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD11	3	0.15
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD12	3	0.15
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD13	3	0.15
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG21	4	0.15
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG22	4	0.15
(1,1520)	1:43:A:ILE:HB	1:52:A:THR:HG23	4	0.15
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	6	0.15
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	6	0.15
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	11	0.15
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	11	0.15
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	11	0.15
(1,1479)	1:110:A:THR:HG21	1:112:A:ILE:HB	9	0.15
(1,1479)	1:110:A:THR:HG22	1:112:A:ILE:HB	9	0.15
(1,1479)	1:110:A:THR:HG23	1:112:A:ILE:HB	9	0.15
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	1	0.15
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	1	0.15
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	1	0.15
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG21	12	0.15
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG22	12	0.15
(1,1416)	1:81:A:GLN:HA	1:111:A:VAL:HG23	12	0.15
(1,1340)	1:38:A:GLY:HA2	1:39:A:ARG:HB3	10	0.15
(1,1318)	1:96:A:LEU:HD21	1:100:A:SER:HA	14	0.15
(1,1318)	1:96:A:LEU:HD22	1:100:A:SER:HA	14	0.15
(1,1318)	1:96:A:LEU:HD23	1:100:A:SER:HA	14	0.15
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	15	0.15
(1,1231)	1:105:A:ILE:HG21	1:113:A:TRP:HE3	12	0.15
(1,1231)	1:105:A:ILE:HG22	1:113:A:TRP:HE3	12	0.15
(1,1231)	1:105:A:ILE:HG23	1:113:A:TRP:HE3	12	0.15
(1,1217)	1:105:A:ILE:HD11	1:114:A:ASP:HB3	17	0.15
(1,1217)	1:105:A:ILE:HD12	1:114:A:ASP:HB3	17	0.15
(1,1217)	1:105:A:ILE:HD13	1:114:A:ASP:HB3	17	0.15
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	13	0.15
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	13	0.15
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	13	0.15
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	11	0.15
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	11	0.15
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	11	0.15
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	12	0.15
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	18	0.15
(1,1144)	1:10:A:PHE:HA	1:58:A:CYS:HB3	18	0.15
(1,1123)	1:25:A:GLY:H	1:45:A:CYS:HA	18	0.15
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB2	16	0.15
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB3	16	0.15
(1,1050)	1:5:A:PRO:HD3	1:51:A:TRP:HD1	10	0.15
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	2	0.15
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	2	0.15
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	2	0.15
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG11	18	0.15
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG13	18	0.15
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	18	0.15
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	4	0.15
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	4	0.15
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	4	0.15
(1,898)	1:1:A:GLN:H	1:1:A:GLN:HE22	15	0.15
(1,878)	1:64:A:ARG:HA	1:113:A:TRP:HE1	16	0.15
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	6	0.15
(1,844)	1:28:A:LEU:HD11	1:29:A:ASN:H	20	0.15
(1,844)	1:28:A:LEU:HD12	1:29:A:ASN:H	20	0.15
(1,844)	1:28:A:LEU:HD13	1:29:A:ASN:H	20	0.15
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	4	0.15
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	19	0.15
(1,808)	1:4:A:ALA:HA	1:20:A:PHE:H	7	0.15
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	8	0.15
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB2	16	0.15
(1,805)	1:19:A:GLU:H	1:19:A:GLU:HB3	16	0.15
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	11	0.15
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	14	0.15
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	18	0.15
(1,795)	1:18:A:ASP:H	1:19:A:GLU:HG3	14	0.15
(1,734)	1:46:A:LEU:H	1:52:A:THR:H	8	0.15
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	13	0.15
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	13	0.15
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	13	0.15
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	20	0.15
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	20	0.15
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	20	0.15
(1,691)	1:61:A:LYS:H	1:111:A:VAL:H	18	0.15
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	13	0.15
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	1	0.15
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	13	0.15
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	3	0.15
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	3	0.15
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	3	0.15
(1,573)	1:79:A:GLY:H	1:81:A:GLN:H	13	0.15
(1,483)	1:98:A:GLY:HA2	1:100:A:SER:H	4	0.15
(1,483)	1:98:A:GLY:HA2	1:100:A:SER:H	13	0.15
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	2	0.15
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	15	0.15
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	9	0.15
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD11	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD12	4	0.15
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD13	4	0.15
(1,430)	1:117:A:THR:H	1:119:A:ILE:HG13	10	0.15
(1,373)	1:13:A:PRO:HB3	1:30:A:TYR:H	20	0.15
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	10	0.15
(1,273)	1:10:A:PHE:HD1	1:33:A:ARG:H	4	0.15
(1,273)	1:10:A:PHE:HD2	1:33:A:ARG:H	4	0.15
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	2	0.15
(1,259)	1:15:A:GLN:H	1:17:A:THR:HG21	1	0.15
(1,259)	1:15:A:GLN:H	1:17:A:THR:HG22	1	0.15
(1,259)	1:15:A:GLN:H	1:17:A:THR:HG23	1	0.15
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	3	0.15
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	13	0.15
(1,180)	1:38:A:GLY:HA3	1:58:A:CYS:H	15	0.15
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	5	0.15
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	16	0.15
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	16	0.15
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	6	0.15
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	6	0.15
(1,149)	1:92:A:LYS:HB3	1:93:A:GLY:H	20	0.15
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	7	0.15
(1,133)	1:79:A:GLY:H	1:80:A:ILE:H	12	0.15
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	5	0.15
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	13	0.15
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	6	0.15
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	19	0.15
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	10	0.15
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	15	0.15
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	5	0.15
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	5	0.15
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	5	0.15
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	13	0.15
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	13	0.15
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	13	0.15
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	18	0.15
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	18	0.15
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	18	0.15
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	8	0.14
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	8	0.14
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	8	0.14
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	8	0.14
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	11	0.14
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	11	0.14
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	11	0.14
(1,2535)	1:99:A:SER:HB2	1:115:A:GLN:HA	7	0.14
(1,2535)	1:99:A:SER:HB3	1:115:A:GLN:HA	7	0.14
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	13	0.14
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	13	0.14
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	13	0.14
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	13	0.14
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	13	0.14
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	13	0.14
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	6	0.14
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	6	0.14
(1,2490)	1:95:A:ARG:HG2	1:121:A:ASP:H	18	0.14
(1,2490)	1:95:A:ARG:HG3	1:121:A:ASP:H	18	0.14
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	3	0.14
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	3	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	11	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	11	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	11	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	11	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	11	0.14
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	11	0.14
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	11	0.14
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	5	0.14
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	5	0.14
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	5	0.14
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	5	0.14
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	7	0.14
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	7	0.14
(1,2420)	1:82:A:PHE:HD1	1:104:A:CYS:HB2	12	0.14
(1,2420)	1:82:A:PHE:HD1	1:104:A:CYS:HB3	12	0.14
(1,2420)	1:82:A:PHE:HD2	1:104:A:CYS:HB2	12	0.14
(1,2420)	1:82:A:PHE:HD2	1:104:A:CYS:HB3	12	0.14
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	16	0.14
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	16	0.14
(1,2395)	1:76:A:VAL:HG11	1:113:A:TRP:HZ2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:76:A:VAL:HG12	1:113:A:TRP:HZ2	10	0.14
(1,2395)	1:76:A:VAL:HG13	1:113:A:TRP:HZ2	10	0.14
(1,2395)	1:76:A:VAL:HG21	1:113:A:TRP:HZ2	10	0.14
(1,2395)	1:76:A:VAL:HG22	1:113:A:TRP:HZ2	10	0.14
(1,2395)	1:76:A:VAL:HG23	1:113:A:TRP:HZ2	10	0.14
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	2	0.14
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	3	0.14
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	3	0.14
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	3	0.14
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	3	0.14
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	3	0.14
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	3	0.14
(1,2364)	1:73:A:MET:HG2	1:91:A:THR:H	18	0.14
(1,2364)	1:73:A:MET:HG3	1:91:A:THR:H	18	0.14
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	3	0.14
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	3	0.14
(1,2354)	1:71:A:ASN:HB2	1:91:A:THR:H	8	0.14
(1,2354)	1:71:A:ASN:HB3	1:91:A:THR:H	8	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG11	16	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG12	16	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG13	16	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG21	16	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG22	16	0.14
(1,2339)	1:69:A:PRO:HD2	1:74:A:VAL:HG23	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG11	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG12	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG13	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG21	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG22	16	0.14
(1,2339)	1:69:A:PRO:HD3	1:74:A:VAL:HG23	16	0.14
(1,2311)	1:65:A:ASN:HB2	1:67:A:PRO:HG2	9	0.14
(1,2311)	1:65:A:ASN:HB3	1:67:A:PRO:HG2	9	0.14
(1,2297)	1:63:A:CYS:HB2	1:113:A:TRP:HE1	1	0.14
(1,2297)	1:63:A:CYS:HB3	1:113:A:TRP:HE1	1	0.14
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD2	11	0.14
(1,2287)	1:63:A:CYS:HA	1:64:A:ARG:HD3	11	0.14
(1,2245)	1:60:A:ARG:HG2	1:82:A:PHE:HB3	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2245)	1:60:A:ARG:HG3	1:82:A:PHE:HB3	16	0.14
(1,2221)	1:57:A:ARG:HG2	1:58:A:CYS:H	2	0.14
(1,2221)	1:57:A:ARG:HG3	1:58:A:CYS:H	2	0.14
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	1	0.14
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	1	0.14
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	5	0.14
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	5	0.14
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	20	0.14
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	20	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	5	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	5	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	5	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	5	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	5	0.14
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	5	0.14
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	5	0.14
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD11	1:30:A:TYR:HD2	6	0.14
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD12	1:30:A:TYR:HD2	6	0.14
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD13	1:30:A:TYR:HD2	6	0.14
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD21	1:30:A:TYR:HD2	6	0.14
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD22	1:30:A:TYR:HD2	6	0.14
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD1	6	0.14
(1,2061)	1:16:A:LEU:HD23	1:30:A:TYR:HD2	6	0.14
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB2	2	0.14
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB3	2	0.14
(1,1952)	1:36:A:TYR:HE1	1:61:A:LYS:H	11	0.14
(1,1952)	1:36:A:TYR:HE2	1:61:A:LYS:H	11	0.14
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	4	0.14
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	13	0.14
(1,1918)	1:2:A:CYS:HB2	1:5:A:PRO:HB3	15	0.14
(1,1902)	1:24:A:ILE:HA	1:49:A:SER:HA	14	0.14
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB1	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB2	9	0.14
(1,1884)	1:8:A:LEU:HD11	1:11:A:ALA:HB3	9	0.14
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB1	9	0.14
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB2	9	0.14
(1,1884)	1:8:A:LEU:HD12	1:11:A:ALA:HB3	9	0.14
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB1	9	0.14
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB2	9	0.14
(1,1884)	1:8:A:LEU:HD13	1:11:A:ALA:HB3	9	0.14
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	13	0.14
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	16	0.14
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	8	0.14
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	8	0.14
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	8	0.14
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	8	0.14
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	8	0.14
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	8	0.14
(1,1850)	1:99:A:SER:HB2	1:115:A:GLN:HA	4	0.14
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	16	0.14
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	8	0.14
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	8	0.14
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	8	0.14
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	2	0.14
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	12	0.14
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	12	0.14
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	12	0.14
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD11	20	0.14
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD12	20	0.14
(1,1768)	1:23:A:PRO:HB2	1:24:A:ILE:HD13	20	0.14
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD11	20	0.14
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD12	20	0.14
(1,1768)	1:23:A:PRO:HB3	1:24:A:ILE:HD13	20	0.14
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	3	0.14
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	3	0.14
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	3	0.14
(1,1732)	1:27:A:TYR:HA	1:44:A:ILE:HB	10	0.14
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	14	0.14
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG21	7	0.14
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG22	7	0.14
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG23	7	0.14
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG21	7	0.14
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG22	7	0.14
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG21	7	0.14
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG22	7	0.14
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG23	7	0.14
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	4	0.14
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	7	0.14
(1,1656)	1:111:A:VAL:HA	1:112:A:ILE:HG21	13	0.14
(1,1656)	1:111:A:VAL:HA	1:112:A:ILE:HG22	13	0.14
(1,1656)	1:111:A:VAL:HA	1:112:A:ILE:HG23	13	0.14
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	9	0.14
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	9	0.14
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	9	0.14
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	19	0.14
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	10	0.14
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	10	0.14
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	4	0.14
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	4	0.14
(1,1581)	1:5:A:PRO:HG2	1:6:A:GLU:HA	8	0.14
(1,1581)	1:5:A:PRO:HG3	1:6:A:GLU:HA	8	0.14
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	2	0.14
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	2	0.14
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	2	0.14
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	4	0.14
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	4	0.14
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	4	0.14
(1,1535)	1:105:A:ILE:HD11	1:115:A:GLN:H	2	0.14
(1,1535)	1:105:A:ILE:HD12	1:115:A:GLN:H	2	0.14
(1,1535)	1:105:A:ILE:HD13	1:115:A:GLN:H	2	0.14
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG21	19	0.14
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG22	19	0.14
(1,1518)	1:51:A:TRP:HB3	1:52:A:THR:HG23	19	0.14
(1,1486)	1:44:A:ILE:HD11	1:52:A:THR:HA	20	0.14
(1,1486)	1:44:A:ILE:HD12	1:52:A:THR:HA	20	0.14
(1,1486)	1:44:A:ILE:HD13	1:52:A:THR:HA	20	0.14
(1,1462)	1:96:A:LEU:HG	1:119:A:ILE:HB	11	0.14
(1,1459)	1:62:A:SER:HA	1:111:A:VAL:HG11	11	0.14
(1,1459)	1:62:A:SER:HA	1:111:A:VAL:HG12	11	0.14
(1,1459)	1:62:A:SER:HA	1:111:A:VAL:HG13	11	0.14
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	11	0.14
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	11	0.14
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	11	0.14
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	16	0.14
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	16	0.14
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD11	17	0.14
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD12	17	0.14
(1,1385)	1:74:A:VAL:HB	1:86:A:ILE:HD13	17	0.14
(1,1384)	1:80:A:ILE:HG21	1:86:A:ILE:HD11	12	0.14
(1,1384)	1:80:A:ILE:HG21	1:86:A:ILE:HD12	12	0.14
(1,1384)	1:80:A:ILE:HG21	1:86:A:ILE:HD13	12	0.14
(1,1384)	1:80:A:ILE:HG22	1:86:A:ILE:HD11	12	0.14
(1,1384)	1:80:A:ILE:HG22	1:86:A:ILE:HD12	12	0.14
(1,1384)	1:80:A:ILE:HG22	1:86:A:ILE:HD13	12	0.14
(1,1384)	1:80:A:ILE:HG23	1:86:A:ILE:HD11	12	0.14
(1,1384)	1:80:A:ILE:HG23	1:86:A:ILE:HD12	12	0.14
(1,1384)	1:80:A:ILE:HG23	1:86:A:ILE:HD13	12	0.14
(1,1363)	1:5:A:PRO:HD2	1:20:A:PHE:H	3	0.14
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB1	16	0.14
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB2	16	0.14
(1,1332)	1:8:A:LEU:H	1:11:A:ALA:HB3	16	0.14
(1,1327)	1:60:A:ARG:HD2	1:82:A:PHE:HD1	14	0.14
(1,1327)	1:60:A:ARG:HD2	1:82:A:PHE:HD2	14	0.14
(1,1314)	1:88:A:TYR:HB3	1:96:A:LEU:HG	19	0.14
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	4	0.14
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	17	0.14
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	19	0.14
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	19	0.14
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	19	0.14
(1,1283)	1:24:A:ILE:HD11	1:25:A:GLY:H	13	0.14
(1,1283)	1:24:A:ILE:HD12	1:25:A:GLY:H	13	0.14
(1,1283)	1:24:A:ILE:HD13	1:25:A:GLY:H	13	0.14
(1,1269)	1:14:A:THR:HG21	1:29:A:ASN:H	16	0.14
(1,1269)	1:14:A:THR:HG22	1:29:A:ASN:H	16	0.14
(1,1269)	1:14:A:THR:HG23	1:29:A:ASN:H	16	0.14
(1,1223)	1:94:A:TYR:HD1	1:121:A:ASP:HA	20	0.14
(1,1223)	1:94:A:TYR:HD2	1:121:A:ASP:HA	20	0.14
(1,1219)	1:117:A:THR:HG21	1:119:A:ILE:HA	1	0.14
(1,1219)	1:117:A:THR:HG22	1:119:A:ILE:HA	1	0.14
(1,1219)	1:117:A:THR:HG23	1:119:A:ILE:HA	1	0.14
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	4	0.14
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	4	0.14
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	4	0.14
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	14	0.14
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	14	0.14
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	18	0.14
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	19	0.14
(1,1142)	1:10:A:PHE:HE1	1:57:A:ARG:HB3	8	0.14
(1,1142)	1:10:A:PHE:HE2	1:57:A:ARG:HB3	8	0.14
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB2	6	0.14
(1,1100)	1:18:A:ASP:H	1:19:A:GLU:HB3	6	0.14
(1,1096)	1:17:A:THR:HG21	1:19:A:GLU:HG3	12	0.14
(1,1096)	1:17:A:THR:HG22	1:19:A:GLU:HG3	12	0.14
(1,1096)	1:17:A:THR:HG23	1:19:A:GLU:HG3	12	0.14
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG21	15	0.14
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG22	15	0.14
(1,1090)	1:16:A:LEU:HA	1:17:A:THR:HG23	15	0.14
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	12	0.14
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	12	0.14
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	12	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	10	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	10	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	10	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	10	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	10	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	10	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	10	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	10	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	10	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	20	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	20	0.14
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	20	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	20	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	20	0.14
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	20	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	20	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	20	0.14
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	20	0.14
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD11	18	0.14
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD12	18	0.14
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD13	18	0.14
(1,1024)	1:76:A:VAL:HB	1:80:A:ILE:HD11	12	0.14
(1,1024)	1:76:A:VAL:HB	1:80:A:ILE:HD12	12	0.14
(1,1024)	1:76:A:VAL:HB	1:80:A:ILE:HD13	12	0.14
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	9	0.14
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	9	0.14
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:81:A:GLN:HB2	1:81:A:GLN:HE21	4	0.14
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	18	0.14
(1,927)	1:65:A:ASN:HD21	1:68:A:ASP:HA	5	0.14
(1,904)	1:1:A:GLN:HE21	1:23:A:PRO:HD2	10	0.14
(1,904)	1:1:A:GLN:HE21	1:23:A:PRO:HD3	10	0.14
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	9	0.14
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	9	0.14
(1,874)	1:7:A:TRP:HE1	1:9:A:PRO:HA	18	0.14
(1,873)	1:7:A:TRP:HE1	1:8:A:LEU:H	2	0.14
(1,871)	1:47:A:LYS:H	1:51:A:TRP:H	1	0.14
(1,864)	1:27:A:TYR:HE1	1:42:A:SER:H	6	0.14
(1,864)	1:27:A:TYR:HE2	1:42:A:SER:H	6	0.14
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	14	0.14
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	10	0.14
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	14	0.14
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	11	0.14
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	3	0.14
(1,810)	1:19:A:GLU:HG2	1:20:A:PHE:H	5	0.14
(1,809)	1:19:A:GLU:HG3	1:20:A:PHE:H	12	0.14
(1,806)	1:18:A:ASP:H	1:20:A:PHE:H	4	0.14
(1,803)	1:19:A:GLU:H	1:19:A:GLU:HG3	15	0.14
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	12	0.14
(1,786)	1:15:A:GLN:HB2	1:16:A:LEU:H	2	0.14
(1,781)	1:15:A:GLN:HB2	1:17:A:THR:H	14	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	11	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	11	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	11	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	19	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	19	0.14
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	19	0.14
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	12	0.14
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	14	0.14
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	4	0.14
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	19	0.14
(1,651)	1:73:A:MET:HA	1:74:A:VAL:H	17	0.14
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD1	11	0.14
(1,650)	1:74:A:VAL:H	1:88:A:TYR:HD2	11	0.14
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	15	0.14
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	15	0.14
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	15	0.14
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD11	8	0.14
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD12	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	1:64:A:ARG:H	1:80:A:ILE:HD13	8	0.14
(1,598)	1:64:A:ARG:H	1:113:A:TRP:HD1	19	0.14
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	19	0.14
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	8	0.14
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	19	0.14
(1,491)	1:98:A:GLY:H	1:119:A:ILE:HG12	8	0.14
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB2	17	0.14
(1,472)	1:99:A:SER:H	1:115:A:GLN:HB3	17	0.14
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	7	0.14
(1,425)	1:102:A:ALA:HB1	1:116:A:GLU:H	4	0.14
(1,425)	1:102:A:ALA:HB2	1:116:A:GLU:H	4	0.14
(1,425)	1:102:A:ALA:HB3	1:116:A:GLU:H	4	0.14
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	5	0.14
(1,401)	1:102:A:ALA:HA	1:115:A:GLN:H	3	0.14
(1,401)	1:102:A:ALA:HA	1:115:A:GLN:H	16	0.14
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	6	0.14
(1,381)	1:119:A:ILE:HG13	1:120:A:CYS:H	11	0.14
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	6	0.14
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	6	0.14
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	2	0.14
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	19	0.14
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	17	0.14
(1,228)	1:111:A:VAL:HG21	1:113:A:TRP:H	18	0.14
(1,228)	1:111:A:VAL:HG22	1:113:A:TRP:H	18	0.14
(1,228)	1:111:A:VAL:HG23	1:113:A:TRP:H	18	0.14
(1,192)	1:106:A:ILE:HG21	1:110:A:THR:H	10	0.14
(1,192)	1:106:A:ILE:HG22	1:110:A:THR:H	10	0.14
(1,192)	1:106:A:ILE:HG23	1:110:A:THR:H	10	0.14
(1,187)	1:88:A:TYR:HB2	1:119:A:ILE:H	11	0.14
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	5	0.14
(1,183)	1:99:A:SER:H	1:119:A:ILE:H	10	0.14
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	15	0.14
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	15	0.14
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	15	0.14
(1,161)	1:14:A:THR:H	1:29:A:ASN:H	17	0.14
(1,160)	1:14:A:THR:H	1:30:A:TYR:H	8	0.14
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	4	0.14
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	2	0.14
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	13	0.14
(1,88)	1:96:A:LEU:HD11	1:97:A:ILE:H	3	0.14
(1,88)	1:96:A:LEU:HD12	1:97:A:ILE:H	3	0.14
(1,88)	1:96:A:LEU:HD13	1:97:A:ILE:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:96:A:LEU:HD11	1:97:A:ILE:H	20	0.14
(1,88)	1:96:A:LEU:HD12	1:97:A:ILE:H	20	0.14
(1,88)	1:96:A:LEU:HD13	1:97:A:ILE:H	20	0.14
(1,79)	1:58:A:CYS:HB3	1:60:A:ARG:H	18	0.14
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	3	0.14
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	12	0.14
(1,2561)	1:109:A:ASP:HB2	1:110:A:THR:HB	1	0.13
(1,2561)	1:109:A:ASP:HB3	1:110:A:THR:HB	1	0.13
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	2	0.13
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	2	0.13
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	2	0.13
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	2	0.13
(1,2507)	1:96:A:LEU:HD11	1:100:A:SER:HA	6	0.13
(1,2507)	1:96:A:LEU:HD12	1:100:A:SER:HA	6	0.13
(1,2507)	1:96:A:LEU:HD13	1:100:A:SER:HA	6	0.13
(1,2507)	1:96:A:LEU:HD21	1:100:A:SER:HA	6	0.13
(1,2507)	1:96:A:LEU:HD22	1:100:A:SER:HA	6	0.13
(1,2507)	1:96:A:LEU:HD23	1:100:A:SER:HA	6	0.13
(1,2492)	1:95:A:ARG:HG2	1:121:A:ASP:HB2	1	0.13
(1,2492)	1:95:A:ARG:HG3	1:121:A:ASP:HB2	1	0.13
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	4	0.13
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	4	0.13
(1,2476)	1:92:A:LYS:HG2	1:93:A:GLY:H	12	0.13
(1,2476)	1:92:A:LYS:HG3	1:93:A:GLY:H	12	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	2	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	2	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD11	9	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD12	9	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD13	9	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD21	9	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD22	9	0.13
(1,2464)	1:90:A:CYS:HB2	1:96:A:LEU:HD23	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD11	9	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD12	9	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD13	9	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD21	9	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD22	9	0.13
(1,2464)	1:90:A:CYS:HB3	1:96:A:LEU:HD23	9	0.13
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB2	4	0.13
(1,2450)	1:87:A:LYS:HD2	1:101:A:SER:HB3	4	0.13
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB2	4	0.13
(1,2450)	1:87:A:LYS:HD3	1:101:A:SER:HB3	4	0.13
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	18	0.13
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	18	0.13
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	20	0.13
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	20	0.13
(1,2432)	1:85:A:GLN:HA	1:101:A:SER:HB2	8	0.13
(1,2432)	1:85:A:GLN:HA	1:101:A:SER:HB3	8	0.13
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	4	0.13
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	4	0.13
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	12	0.13
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	12	0.13
(1,2337)	1:69:A:PRO:HD2	1:74:A:VAL:HA	11	0.13
(1,2337)	1:69:A:PRO:HD3	1:74:A:VAL:HA	11	0.13
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	4	0.13
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	4	0.13
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	10	0.13
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	10	0.13
(1,2328)	1:68:A:ASP:HB2	1:73:A:MET:H	15	0.13
(1,2328)	1:68:A:ASP:HB3	1:73:A:MET:H	15	0.13
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG21	2	0.13
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG22	2	0.13
(1,2313)	1:65:A:ASN:HB2	1:80:A:ILE:HG23	2	0.13
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG21	2	0.13
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG22	2	0.13
(1,2313)	1:65:A:ASN:HB3	1:80:A:ILE:HG23	2	0.13
(1,2304)	1:64:A:ARG:HD2	1:113:A:TRP:HD1	3	0.13
(1,2304)	1:64:A:ARG:HD3	1:113:A:TRP:HD1	3	0.13
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD2	7	0.13
(1,2299)	1:64:A:ARG:HA	1:64:A:ARG:HD3	7	0.13
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	6	0.13
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	6	0.13
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	6	0.13
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	8	0.13
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	8	0.13
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	8	0.13
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	8	0.13
(1,2249)	1:60:A:ARG:HD2	1:81:A:GLN:HE21	20	0.13
(1,2249)	1:60:A:ARG:HD3	1:81:A:GLN:HE21	20	0.13
(1,2242)	1:60:A:ARG:HG2	1:81:A:GLN:HE21	9	0.13
(1,2242)	1:60:A:ARG:HG3	1:81:A:GLN:HE21	9	0.13
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	14	0.13
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	14	0.13
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	16	0.13
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	16	0.13
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	2	0.13
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	2	0.13
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	2	0.13
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	2	0.13
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	16	0.13
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	16	0.13
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	16	0.13
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	16	0.13
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	16	0.13
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	16	0.13
(1,2165)	1:47:A:LYS:HG2	1:49:A:SER:H	19	0.13
(1,2165)	1:47:A:LYS:HG3	1:49:A:SER:H	19	0.13
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	20	0.13
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	20	0.13
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	20	0.13
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	20	0.13
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	20	0.13
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	20	0.13
(1,2135)	1:41:A:PHE:HB2	1:43:A:ILE:H	17	0.13
(1,2135)	1:41:A:PHE:HB3	1:43:A:ILE:H	17	0.13
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD2	17	0.13
(1,2131)	1:39:A:ARG:HD2	1:40:A:PRO:HD3	17	0.13
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD2	17	0.13
(1,2131)	1:39:A:ARG:HD3	1:40:A:PRO:HD3	17	0.13
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	6	0.13
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	6	0.13
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	6	0.13
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	6	0.13
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	6	0.13
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD11	2	0.13
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD12	2	0.13
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD13	2	0.13
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD21	2	0.13
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD22	2	0.13
(1,2051)	1:16:A:LEU:H	1:16:A:LEU:HD23	2	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD11	4	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD12	4	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD13	4	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD21	4	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD22	4	0.13
(1,2048)	1:15:A:GLN:HE21	1:28:A:LEU:HD23	4	0.13
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB2	1	0.13
(1,2040)	1:13:A:PRO:HA	1:31:A:GLU:HB3	1	0.13
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE1	8	0.13
(1,1975)	1:8:A:LEU:HG	1:30:A:TYR:HE2	8	0.13
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE1	7	0.13
(1,1974)	1:5:A:PRO:HD2	1:30:A:TYR:HE2	7	0.13
(1,1959)	1:43:A:ILE:HB	1:51:A:TRP:HD1	5	0.13
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE1	20	0.13
(1,1956)	1:60:A:ARG:HA	1:82:A:PHE:HE2	20	0.13
(1,1947)	1:36:A:TYR:HE1	1:59:A:ARG:HA	10	0.13
(1,1947)	1:36:A:TYR:HE2	1:59:A:ARG:HA	10	0.13
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	10	0.13
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	11	0.13
(1,1935)	1:68:A:ASP:HA	1:74:A:VAL:HB	19	0.13
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	8	0.13
(1,1919)	1:5:A:PRO:HB3	1:43:A:ILE:HB	20	0.13
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD11	6	0.13
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD12	6	0.13
(1,1905)	1:5:A:PRO:HB2	1:43:A:ILE:HD13	6	0.13
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	8	0.13
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	12	0.13
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	12	0.13
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	12	0.13
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	12	0.13
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	12	0.13
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	12	0.13
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB2	1	0.13
(1,1849)	1:99:A:SER:HB2	1:115:A:GLN:HB3	1	0.13
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	4	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	9	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	9	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	15	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	15	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	15	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	16	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	16	0.13
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	16	0.13
(1,1815)	1:73:A:MET:HE1	1:90:A:CYS:HA	7	0.13
(1,1815)	1:73:A:MET:HE2	1:90:A:CYS:HA	7	0.13
(1,1815)	1:73:A:MET:HE3	1:90:A:CYS:HA	7	0.13
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	14	0.13
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	14	0.13
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	14	0.13
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG21	13	0.13
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG22	13	0.13
(1,1783)	1:27:A:TYR:HB3	1:44:A:ILE:HG23	13	0.13
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	5	0.13
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	5	0.13
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	5	0.13
(1,1759)	1:106:A:ILE:HB	1:107:A:SER:HA	8	0.13
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	16	0.13
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	16	0.13
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	16	0.13
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	2	0.13
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	2	0.13
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	7	0.13
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	7	0.13
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	7	0.13
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	7	0.13
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	7	0.13
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	7	0.13
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	9	0.13
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	9	0.13
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	9	0.13
(1,1730)	1:85:A:GLN:HB2	1:113:A:TRP:HZ3	4	0.13
(1,1730)	1:85:A:GLN:HB2	1:113:A:TRP:HZ3	14	0.13
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	15	0.13
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	3	0.13
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	15	0.13
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	15	0.13
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD1	11	0.13
(1,1636)	1:74:A:VAL:HA	1:88:A:TYR:HD2	11	0.13
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	10	0.13
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	8	0.13
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	8	0.13
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	7	0.13
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	7	0.13
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	7	0.13
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	1	0.13
(1,1535)	1:105:A:ILE:HD11	1:115:A:GLN:H	12	0.13
(1,1535)	1:105:A:ILE:HD12	1:115:A:GLN:H	12	0.13
(1,1535)	1:105:A:ILE:HD13	1:115:A:GLN:H	12	0.13
(1,1525)	1:16:A:LEU:HB2	1:28:A:LEU:HG	15	0.13
(1,1525)	1:16:A:LEU:HB3	1:28:A:LEU:HG	15	0.13
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	8	0.13
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	8	0.13
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	8	0.13
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	17	0.13
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	17	0.13
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	17	0.13
(1,1453)	1:63:A:CYS:HA	1:64:A:ARG:HB3	5	0.13
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	14	0.13
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	14	0.13
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	14	0.13
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	3	0.13
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	11	0.13
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD11	20	0.13
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD12	20	0.13
(1,1381)	1:85:A:GLN:HG2	1:86:A:ILE:HD13	20	0.13
(1,1376)	1:65:A:ASN:HD21	1:86:A:ILE:HD11	2	0.13
(1,1376)	1:65:A:ASN:HD21	1:86:A:ILE:HD12	2	0.13
(1,1376)	1:65:A:ASN:HD21	1:86:A:ILE:HD13	2	0.13
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	14	0.13
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	14	0.13
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	15	0.13
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	15	0.13
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	20	0.13
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	20	0.13
(1,1320)	1:88:A:TYR:HB3	1:96:A:LEU:HD21	3	0.13
(1,1320)	1:88:A:TYR:HB3	1:96:A:LEU:HD22	3	0.13
(1,1320)	1:88:A:TYR:HB3	1:96:A:LEU:HD23	3	0.13
(1,1318)	1:96:A:LEU:HD21	1:100:A:SER:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:96:A:LEU:HD22	1:100:A:SER:HA	6	0.13
(1,1318)	1:96:A:LEU:HD23	1:100:A:SER:HA	6	0.13
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	5	0.13
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	5	0.13
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	5	0.13
(1,1259)	1:27:A:TYR:H	1:27:A:TYR:HE1	10	0.13
(1,1259)	1:27:A:TYR:H	1:27:A:TYR:HE2	10	0.13
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	7	0.13
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	12	0.13
(1,1231)	1:105:A:ILE:HG21	1:113:A:TRP:HE3	20	0.13
(1,1231)	1:105:A:ILE:HG22	1:113:A:TRP:HE3	20	0.13
(1,1231)	1:105:A:ILE:HG23	1:113:A:TRP:HE3	20	0.13
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG21	12	0.13
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG22	12	0.13
(1,1210)	1:85:A:GLN:HG2	1:103:A:THR:HG23	12	0.13
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	19	0.13
(1,1144)	1:10:A:PHE:HA	1:58:A:CYS:HB3	13	0.13
(1,1121)	1:44:A:ILE:H	1:44:A:ILE:HG13	12	0.13
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	10	0.13
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	10	0.13
(1,1044)	1:2:A:CYS:HB2	1:51:A:TRP:HD1	11	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	2	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	2	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	2	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	7	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	7	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	7	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD11	13	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD12	13	0.13
(1,1025)	1:76:A:VAL:HA	1:80:A:ILE:HD13	13	0.13
(1,1019)	1:44:A:ILE:HD11	1:51:A:TRP:HB3	12	0.13
(1,1019)	1:44:A:ILE:HD12	1:51:A:TRP:HB3	12	0.13
(1,1019)	1:44:A:ILE:HD13	1:51:A:TRP:HB3	12	0.13
(1,1005)	1:43:A:ILE:HG21	1:52:A:THR:HA	1	0.13
(1,1005)	1:43:A:ILE:HG22	1:52:A:THR:HA	1	0.13
(1,1005)	1:43:A:ILE:HG23	1:52:A:THR:HA	1	0.13
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG21	14	0.13
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG22	14	0.13
(1,1003)	1:61:A:LYS:HB2	1:111:A:VAL:HG23	14	0.13
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	1	0.13
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	1	0.13
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:68:A:ASP:H	1:69:A:PRO:HA	1	0.13
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	8	0.13
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	17	0.13
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD11	13	0.13
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD12	13	0.13
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD13	13	0.13
(1,914)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	16	0.13
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	13	0.13
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	13	0.13
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	13	0.13
(1,891)	1:3:A:ASN:H	1:3:A:ASN:HD22	15	0.13
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	19	0.13
(1,887)	1:4:A:ALA:HB1	1:51:A:TRP:HE1	1	0.13
(1,887)	1:4:A:ALA:HB2	1:51:A:TRP:HE1	1	0.13
(1,887)	1:4:A:ALA:HB3	1:51:A:TRP:HE1	1	0.13
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	20	0.13
(1,839)	1:15:A:GLN:HE22	1:29:A:ASN:H	17	0.13
(1,812)	1:4:A:ALA:H	1:21:A:GLU:H	7	0.13
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	19	0.13
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	19	0.13
(1,741)	1:45:A:CYS:HA	1:52:A:THR:H	8	0.13
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD11	18	0.13
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD12	18	0.13
(1,722)	1:6:A:GLU:H	1:43:A:ILE:HD13	18	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	6	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	6	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	6	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	13	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	13	0.13
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	13	0.13
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	12	0.13
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	3	0.13
(1,583)	1:26:A:THR:H	1:51:A:TRP:HH2	2	0.13
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	14	0.13
(1,565)	1:74:A:VAL:HB	1:87:A:LYS:H	20	0.13
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	9	0.13
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	14	0.13
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	4	0.13
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	10	0.13
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	15	0.13
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	3	0.13
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:106:A:ILE:HG21	1:109:A:ASP:H	20	0.13
(1,466)	1:106:A:ILE:HG22	1:109:A:ASP:H	20	0.13
(1,466)	1:106:A:ILE:HG23	1:109:A:ASP:H	20	0.13
(1,461)	1:107:A:SER:HA	1:109:A:ASP:H	15	0.13
(1,447)	1:106:A:ILE:HG21	1:108:A:GLY:H	11	0.13
(1,447)	1:106:A:ILE:HG22	1:108:A:GLY:H	11	0.13
(1,447)	1:106:A:ILE:HG23	1:108:A:GLY:H	11	0.13
(1,429)	1:116:A:GLU:HB2	1:117:A:THR:H	17	0.13
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	17	0.13
(1,377)	1:94:A:TYR:HE1	1:120:A:CYS:H	15	0.13
(1,377)	1:94:A:TYR:HE2	1:120:A:CYS:H	15	0.13
(1,377)	1:94:A:TYR:HE1	1:120:A:CYS:H	17	0.13
(1,377)	1:94:A:TYR:HE2	1:120:A:CYS:H	17	0.13
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE1	11	0.13
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE2	11	0.13
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE1	20	0.13
(1,275)	1:33:A:ARG:H	1:36:A:TYR:HE2	20	0.13
(1,266)	1:43:A:ILE:HG21	1:55:A:LYS:H	4	0.13
(1,266)	1:43:A:ILE:HG22	1:55:A:LYS:H	4	0.13
(1,266)	1:43:A:ILE:HG23	1:55:A:LYS:H	4	0.13
(1,236)	1:113:A:TRP:H	1:113:A:TRP:HE1	8	0.13
(1,223)	1:106:A:ILE:HA	1:112:A:ILE:H	1	0.13
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD11	15	0.13
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD12	15	0.13
(1,190)	1:119:A:ILE:H	1:119:A:ILE:HD13	15	0.13
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	10	0.13
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	8	0.13
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	8	0.13
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD1	13	0.13
(1,162)	1:14:A:THR:H	1:30:A:TYR:HD2	13	0.13
(1,156)	1:93:A:GLY:H	1:94:A:TYR:H	1	0.13
(1,144)	1:89:A:SER:H	1:100:A:SER:HA	19	0.13
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	9	0.13
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	18	0.13
(1,120)	1:69:A:PRO:HB2	1:72:A:GLY:H	12	0.13
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	14	0.13
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD1	9	0.13
(1,84)	1:60:A:ARG:H	1:82:A:PHE:HD2	9	0.13
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	12	0.13
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	8	0.13
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	13	0.13
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	7	0.13
(1,29)	1:37:A:SER:H	1:58:A:CYS:HB3	10	0.13
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG21	20	0.12
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG22	20	0.12
(1,2562)	1:109:A:ASP:HB2	1:110:A:THR:HG23	20	0.12
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG21	20	0.12
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG22	20	0.12
(1,2562)	1:109:A:ASP:HB3	1:110:A:THR:HG23	20	0.12
(1,2561)	1:109:A:ASP:HB2	1:110:A:THR:HB	8	0.12
(1,2561)	1:109:A:ASP:HB3	1:110:A:THR:HB	8	0.12
(1,2561)	1:109:A:ASP:HB2	1:110:A:THR:HB	17	0.12
(1,2561)	1:109:A:ASP:HB3	1:110:A:THR:HB	17	0.12
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB2	11	0.12
(1,2536)	1:99:A:SER:HB2	1:115:A:GLN:HB3	11	0.12
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB2	11	0.12
(1,2536)	1:99:A:SER:HB3	1:115:A:GLN:HB3	11	0.12
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG2	8	0.12
(1,2531)	1:99:A:SER:H	1:116:A:GLU:HG3	8	0.12
(1,2515)	1:96:A:LEU:HD11	1:120:A:CYS:H	12	0.12
(1,2515)	1:96:A:LEU:HD12	1:120:A:CYS:H	12	0.12
(1,2515)	1:96:A:LEU:HD13	1:120:A:CYS:H	12	0.12
(1,2515)	1:96:A:LEU:HD21	1:120:A:CYS:H	12	0.12
(1,2515)	1:96:A:LEU:HD22	1:120:A:CYS:H	12	0.12
(1,2515)	1:96:A:LEU:HD23	1:120:A:CYS:H	12	0.12
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD11	1:100:A:SER:HB3	6	0.12
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD12	1:100:A:SER:HB3	6	0.12
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD13	1:100:A:SER:HB3	6	0.12
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD21	1:100:A:SER:HB3	6	0.12
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD22	1:100:A:SER:HB3	6	0.12
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB2	6	0.12
(1,2508)	1:96:A:LEU:HD23	1:100:A:SER:HB3	6	0.12
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB2	7	0.12
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB3	7	0.12
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB2	6	0.12
(1,2485)	1:94:A:TYR:HD1	1:122:A:ARG:HB3	6	0.12
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB2	6	0.12
(1,2485)	1:94:A:TYR:HD2	1:122:A:ARG:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	18	0.12
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	18	0.12
(1,2479)	1:92:A:LYS:HD2	1:93:A:GLY:HA2	11	0.12
(1,2479)	1:92:A:LYS:HD3	1:93:A:GLY:HA2	11	0.12
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	6	0.12
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	6	0.12
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	6	0.12
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	6	0.12
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB2	19	0.12
(1,2447)	1:87:A:LYS:HG3	1:101:A:SER:HB3	19	0.12
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB2	20	0.12
(1,2445)	1:87:A:LYS:HB3	1:89:A:SER:HB3	20	0.12
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE2	1	0.12
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE3	1	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE2	1	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE3	1	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE2	1	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE3	1	0.12
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE2	14	0.12
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE3	14	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE2	14	0.12
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE3	14	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE2	14	0.12
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE3	14	0.12
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	17	0.12
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	17	0.12
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE2	8	0.12
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE3	8	0.12
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE2	11	0.12
(1,2400)	1:77:A:ILE:HG12	1:87:A:LYS:HE3	11	0.12
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE2	15	0.12
(1,2396)	1:77:A:ILE:HA	1:78:A:LYS:HE3	15	0.12
(1,2392)	1:76:A:VAL:HG11	1:80:A:ILE:H	18	0.12
(1,2392)	1:76:A:VAL:HG12	1:80:A:ILE:H	18	0.12
(1,2392)	1:76:A:VAL:HG13	1:80:A:ILE:H	18	0.12
(1,2392)	1:76:A:VAL:HG21	1:80:A:ILE:H	18	0.12
(1,2392)	1:76:A:VAL:HG22	1:80:A:ILE:H	18	0.12
(1,2392)	1:76:A:VAL:HG23	1:80:A:ILE:H	18	0.12
(1,2387)	1:76:A:VAL:HG11	1:77:A:ILE:H	6	0.12
(1,2387)	1:76:A:VAL:HG12	1:77:A:ILE:H	6	0.12
(1,2387)	1:76:A:VAL:HG13	1:77:A:ILE:H	6	0.12
(1,2387)	1:76:A:VAL:HG21	1:77:A:ILE:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2387)	1:76:A:VAL:HG22	1:77:A:ILE:H	6	0.12
(1,2387)	1:76:A:VAL:HG23	1:77:A:ILE:H	6	0.12
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA2	5	0.12
(1,2332)	1:69:A:PRO:HB2	1:72:A:GLY:HA3	5	0.12
(1,2306)	1:65:A:ASN:H	1:65:A:ASN:HB2	2	0.12
(1,2306)	1:65:A:ASN:H	1:65:A:ASN:HB3	2	0.12
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	15	0.12
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	15	0.12
(1,2295)	1:63:A:CYS:HB2	1:113:A:TRP:H	18	0.12
(1,2295)	1:63:A:CYS:HB3	1:113:A:TRP:H	18	0.12
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	5	0.12
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	5	0.12
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB2	6	0.12
(1,2286)	1:63:A:CYS:H	1:81:A:GLN:HB3	6	0.12
(1,2261)	1:61:A:LYS:HA	1:62:A:SER:HB2	17	0.12
(1,2261)	1:61:A:LYS:HA	1:62:A:SER:HB3	17	0.12
(1,2233)	1:60:A:ARG:H	1:60:A:ARG:HG2	8	0.12
(1,2233)	1:60:A:ARG:H	1:60:A:ARG:HG3	8	0.12
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD2	5	0.12
(1,2224)	1:58:A:CYS:HA	1:59:A:ARG:HD3	5	0.12
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	5	0.12
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	5	0.12
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	5	0.12
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	5	0.12
(1,2205)	1:55:A:LYS:HB2	1:56:A:ASP:H	2	0.12
(1,2205)	1:55:A:LYS:HB3	1:56:A:ASP:H	2	0.12
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD2	16	0.12
(1,2202)	1:55:A:LYS:HA	1:57:A:ARG:HD3	16	0.12
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	1	0.12
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	1	0.12
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	1	0.12
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	1	0.12
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	1	0.12
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	1	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG11	14	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG12	14	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG13	14	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG21	14	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG22	14	0.12
(1,2176)	1:48:A:ASN:HB2	1:50:A:VAL:HG23	14	0.12
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG11	14	0.12
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG12	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG13	14	0.12
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG21	14	0.12
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG22	14	0.12
(1,2176)	1:48:A:ASN:HB3	1:50:A:VAL:HG23	14	0.12
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	4	0.12
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	4	0.12
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	4	0.12
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	4	0.12
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	4	0.12
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	4	0.12
(1,2153)	1:46:A:LEU:HD11	1:52:A:THR:HA	1	0.12
(1,2153)	1:46:A:LEU:HD12	1:52:A:THR:HA	1	0.12
(1,2153)	1:46:A:LEU:HD13	1:52:A:THR:HA	1	0.12
(1,2153)	1:46:A:LEU:HD21	1:52:A:THR:HA	1	0.12
(1,2153)	1:46:A:LEU:HD22	1:52:A:THR:HA	1	0.12
(1,2153)	1:46:A:LEU:HD23	1:52:A:THR:HA	1	0.12
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG2	11	0.12
(1,2122)	1:38:A:GLY:H	1:59:A:ARG:HG3	11	0.12
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD2	9	0.12
(1,2121)	1:37:A:SER:HB2	1:59:A:ARG:HD3	9	0.12
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD2	9	0.12
(1,2121)	1:37:A:SER:HB3	1:59:A:ARG:HD3	9	0.12
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	19	0.12
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	19	0.12
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	19	0.12
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	19	0.12
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	19	0.12
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	19	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	6	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	6	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	16	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	16	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	16	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	16	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	16	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	16	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	18	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	18	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	18	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	18	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	18	0.12
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	18	0.12
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	18	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD11	20	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD12	20	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD13	20	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD21	20	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD22	20	0.12
(1,2085)	1:26:A:THR:HB	1:28:A:LEU:HD23	20	0.12
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	12	0.12
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	12	0.12
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	12	0.12
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	12	0.12
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	7	0.12
(1,2057)	1:16:A:LEU:HD11	1:18:A:ASP:H	10	0.12
(1,2057)	1:16:A:LEU:HD12	1:18:A:ASP:H	10	0.12
(1,2057)	1:16:A:LEU:HD13	1:18:A:ASP:H	10	0.12
(1,2057)	1:16:A:LEU:HD21	1:18:A:ASP:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2057)	1:16:A:LEU:HD22	1:18:A:ASP:H	10	0.12
(1,2057)	1:16:A:LEU:HD23	1:18:A:ASP:H	10	0.12
(1,2056)	1:16:A:LEU:HD11	1:17:A:THR:HB	18	0.12
(1,2056)	1:16:A:LEU:HD12	1:17:A:THR:HB	18	0.12
(1,2056)	1:16:A:LEU:HD13	1:17:A:THR:HB	18	0.12
(1,2056)	1:16:A:LEU:HD21	1:17:A:THR:HB	18	0.12
(1,2056)	1:16:A:LEU:HD22	1:17:A:THR:HB	18	0.12
(1,2056)	1:16:A:LEU:HD23	1:17:A:THR:HB	18	0.12
(1,2038)	1:12:A:ARG:H	1:31:A:GLU:HB2	2	0.12
(1,2038)	1:12:A:ARG:H	1:31:A:GLU:HB3	2	0.12
(1,2018)	1:8:A:LEU:HD11	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD11	1:10:A:PHE:HE2	17	0.12
(1,2018)	1:8:A:LEU:HD12	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD12	1:10:A:PHE:HE2	17	0.12
(1,2018)	1:8:A:LEU:HD13	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD13	1:10:A:PHE:HE2	17	0.12
(1,2018)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	17	0.12
(1,2018)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	17	0.12
(1,2018)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	17	0.12
(1,2018)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	17	0.12
(1,2016)	1:8:A:LEU:HD11	1:10:A:PHE:H	17	0.12
(1,2016)	1:8:A:LEU:HD12	1:10:A:PHE:H	17	0.12
(1,2016)	1:8:A:LEU:HD13	1:10:A:PHE:H	17	0.12
(1,2016)	1:8:A:LEU:HD21	1:10:A:PHE:H	17	0.12
(1,2016)	1:8:A:LEU:HD22	1:10:A:PHE:H	17	0.12
(1,2016)	1:8:A:LEU:HD23	1:10:A:PHE:H	17	0.12
(1,1952)	1:36:A:TYR:HE1	1:61:A:LYS:H	17	0.12
(1,1952)	1:36:A:TYR:HE2	1:61:A:LYS:H	17	0.12
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	7	0.12
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	15	0.12
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	3	0.12
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	9	0.12
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	20	0.12
(1,1835)	1:74:A:VAL:HA	1:87:A:LYS:HB3	3	0.12
(1,1809)	1:24:A:ILE:HG21	1:46:A:LEU:HA	5	0.12
(1,1809)	1:24:A:ILE:HG22	1:46:A:LEU:HA	5	0.12
(1,1809)	1:24:A:ILE:HG23	1:46:A:LEU:HA	5	0.12
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	3	0.12
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG21	5	0.12
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG22	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1785)	1:28:A:LEU:H	1:44:A:ILE:HG23	5	0.12
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	8	0.12
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	8	0.12
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	8	0.12
(1,1759)	1:106:A:ILE:HB	1:107:A:SER:HA	5	0.12
(1,1749)	1:15:A:GLN:HB2	1:29:A:ASN:HB2	8	0.12
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	7	0.12
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	7	0.12
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	7	0.12
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	9	0.12
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	9	0.12
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	9	0.12
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	8	0.12
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	8	0.12
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	5	0.12
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	5	0.12
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	5	0.12
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	5	0.12
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	5	0.12
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	5	0.12
(1,1697)	1:99:A:SER:HB3	1:115:A:GLN:HA	2	0.12
(1,1677)	1:44:A:ILE:HB	1:52:A:THR:HB	1	0.12
(1,1674)	1:69:A:PRO:HG2	1:74:A:VAL:HA	16	0.12
(1,1674)	1:69:A:PRO:HG3	1:74:A:VAL:HA	16	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	8	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	8	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	8	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	16	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	16	0.12
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	16	0.12
(1,1486)	1:44:A:ILE:HD11	1:52:A:THR:HA	8	0.12
(1,1486)	1:44:A:ILE:HD12	1:52:A:THR:HA	8	0.12
(1,1486)	1:44:A:ILE:HD13	1:52:A:THR:HA	8	0.12
(1,1462)	1:96:A:LEU:HG	1:119:A:ILE:HB	17	0.12
(1,1457)	1:65:A:ASN:HB3	1:113:A:TRP:HZ2	13	0.12
(1,1452)	1:2:A:CYS:HB2	1:5:A:PRO:HA	9	0.12
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD11	11	0.12
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD12	11	0.12
(1,1426)	1:118:A:PRO:HA	1:119:A:ILE:HD13	11	0.12
(1,1389)	1:75:A:HIS:HD2	1:87:A:LYS:HB3	5	0.12
(1,1387)	1:43:A:ILE:HD11	1:54:A:ALA:H	20	0.12
(1,1387)	1:43:A:ILE:HD12	1:54:A:ALA:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:43:A:ILE:HD13	1:54:A:ALA:H	20	0.12
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE1	6	0.12
(1,1347)	1:10:A:PHE:HB3	1:36:A:TYR:HE2	6	0.12
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	11	0.12
(1,1283)	1:24:A:ILE:HD11	1:25:A:GLY:H	7	0.12
(1,1283)	1:24:A:ILE:HD12	1:25:A:GLY:H	7	0.12
(1,1283)	1:24:A:ILE:HD13	1:25:A:GLY:H	7	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE1	14	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE2	14	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE1	17	0.12
(1,1265)	1:91:A:THR:HB	1:94:A:TYR:HE2	17	0.12
(1,1254)	1:10:A:PHE:HD1	1:58:A:CYS:HB3	14	0.12
(1,1254)	1:10:A:PHE:HD2	1:58:A:CYS:HB3	14	0.12
(1,1239)	1:28:A:LEU:HG	1:51:A:TRP:HZ2	1	0.12
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	2	0.12
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	5	0.12
(1,1165)	1:75:A:HIS:HB3	1:77:A:ILE:HG12	20	0.12
(1,1061)	1:80:A:ILE:HD11	1:113:A:TRP:HD1	5	0.12
(1,1061)	1:80:A:ILE:HD12	1:113:A:TRP:HD1	5	0.12
(1,1061)	1:80:A:ILE:HD13	1:113:A:TRP:HD1	5	0.12
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	18	0.12
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	18	0.12
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	18	0.12
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	1	0.12
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	1	0.12
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	1	0.12
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	1	0.12
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	1	0.12
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	1	0.12
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	1	0.12
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	1	0.12
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	1	0.12
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD11	7	0.12
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD12	7	0.12
(1,1028)	1:65:A:ASN:H	1:80:A:ILE:HD13	7	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD11	5	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD12	5	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD13	5	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD11	5	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD12	5	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD13	5	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD11	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD12	5	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD13	5	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD11	10	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD12	10	0.12
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD13	10	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD11	10	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD12	10	0.12
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD13	10	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD11	10	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD12	10	0.12
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD13	10	0.12
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	15	0.12
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	15	0.12
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	15	0.12
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG11	16	0.12
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG12	16	0.12
(1,982)	1:61:A:LYS:HE3	1:111:A:VAL:HG13	16	0.12
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	13	0.12
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	13	0.12
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	13	0.12
(1,959)	1:22:A:PHE:H	1:51:A:TRP:HE1	11	0.12
(1,954)	1:68:A:ASP:H	1:69:A:PRO:HA	7	0.12
(1,952)	1:107:A:SER:H	1:110:A:THR:H	1	0.12
(1,946)	1:75:A:HIS:HD2	1:76:A:VAL:H	20	0.12
(1,943)	1:46:A:LEU:H	1:51:A:TRP:H	18	0.12
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD11	4	0.12
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD12	4	0.12
(1,932)	1:65:A:ASN:HD21	1:80:A:ILE:HD13	4	0.12
(1,895)	1:2:A:CYS:HA	1:3:A:ASN:HD21	12	0.12
(1,889)	1:7:A:TRP:HE1	1:9:A:PRO:HB3	13	0.12
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	19	0.12
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	9	0.12
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	17	0.12
(1,816)	1:19:A:GLU:HB2	1:21:A:GLU:H	13	0.12
(1,816)	1:19:A:GLU:HB3	1:21:A:GLU:H	13	0.12
(1,813)	1:19:A:GLU:H	1:21:A:GLU:H	8	0.12
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	5	0.12
(1,795)	1:18:A:ASP:H	1:19:A:GLU:HG3	6	0.12
(1,781)	1:15:A:GLN:HB2	1:17:A:THR:H	15	0.12
(1,781)	1:15:A:GLN:HB2	1:17:A:THR:H	16	0.12
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	1	0.12
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	15	0.12
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	15	0.12
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	18	0.12
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	18	0.12
(1,752)	1:47:A:LYS:H	1:49:A:SER:H	9	0.12
(1,732)	1:24:A:ILE:HG13	1:25:A:GLY:H	6	0.12
(1,671)	1:65:A:ASN:H	1:65:A:ASN:HD21	12	0.12
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	10	0.12
(1,639)	1:45:A:CYS:H	1:51:A:TRP:HB3	13	0.12
(1,637)	1:26:A:THR:HB	1:45:A:CYS:H	14	0.12
(1,576)	1:22:A:PHE:HB3	1:26:A:THR:H	10	0.12
(1,459)	1:108:A:GLY:H	1:109:A:ASP:H	20	0.12
(1,428)	1:116:A:GLU:HB3	1:117:A:THR:H	3	0.12
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	3	0.12
(1,401)	1:102:A:ALA:HA	1:115:A:GLN:H	5	0.12
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	1	0.12
(1,400)	1:102:A:ALA:H	1:115:A:GLN:H	9	0.12
(1,365)	1:29:A:ASN:H	1:30:A:TYR:H	13	0.12
(1,346)	1:82:A:PHE:HA	1:106:A:ILE:H	9	0.12
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	11	0.12
(1,322)	1:1:A:GLN:H	1:22:A:PHE:HA	18	0.12
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	12	0.12
(1,273)	1:10:A:PHE:HD1	1:33:A:ARG:H	19	0.12
(1,273)	1:10:A:PHE:HD2	1:33:A:ARG:H	19	0.12
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	4	0.12
(1,269)	1:10:A:PHE:HB2	1:33:A:ARG:H	17	0.12
(1,254)	1:14:A:THR:HA	1:15:A:GLN:H	17	0.12
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	11	0.12
(1,181)	1:10:A:PHE:HE1	1:58:A:CYS:H	20	0.12
(1,181)	1:10:A:PHE:HE2	1:58:A:CYS:H	20	0.12
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	11	0.12
(1,147)	1:87:A:LYS:HB2	1:89:A:SER:H	18	0.12
(1,141)	1:88:A:TYR:H	1:89:A:SER:H	5	0.12
(1,141)	1:88:A:TYR:H	1:89:A:SER:H	19	0.12
(1,123)	1:8:A:LEU:HD21	1:10:A:PHE:H	17	0.12
(1,123)	1:8:A:LEU:HD22	1:10:A:PHE:H	17	0.12
(1,123)	1:8:A:LEU:HD23	1:10:A:PHE:H	17	0.12
(1,108)	1:46:A:LEU:H	1:49:A:SER:H	7	0.12
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	14	0.12
(1,37)	1:1:A:GLN:HE21	1:2:A:CYS:H	5	0.12
(1,34)	1:2:A:CYS:H	1:22:A:PHE:HB2	18	0.12
(1,24)	1:37:A:SER:H	1:58:A:CYS:HA	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:95:A:ARG:H	1:121:A:ASP:HB3	17	0.12
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	7	0.11
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	7	0.11
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB2	3	0.11
(1,2538)	1:99:A:SER:HB2	1:116:A:GLU:HB3	3	0.11
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB2	3	0.11
(1,2538)	1:99:A:SER:HB3	1:116:A:GLU:HB3	3	0.11
(1,2533)	1:99:A:SER:HB2	1:102:A:ALA:HA	15	0.11
(1,2533)	1:99:A:SER:HB3	1:102:A:ALA:HA	15	0.11
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB2	6	0.11
(1,2495)	1:96:A:LEU:H	1:100:A:SER:HB3	6	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD11	8	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD12	8	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD13	8	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD21	8	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD22	8	0.11
(1,2494)	1:96:A:LEU:H	1:96:A:LEU:HD23	8	0.11
(1,2478)	1:92:A:LYS:HD2	1:93:A:GLY:H	17	0.11
(1,2478)	1:92:A:LYS:HD3	1:93:A:GLY:H	17	0.11
(1,2449)	1:87:A:LYS:HD2	1:101:A:SER:HA	19	0.11
(1,2449)	1:87:A:LYS:HD3	1:101:A:SER:HA	19	0.11
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE2	8	0.11
(1,2438)	1:86:A:ILE:HA	1:87:A:LYS:HE3	8	0.11
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE2	15	0.11
(1,2434)	1:85:A:GLN:HG2	1:87:A:LYS:HE3	15	0.11
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD11	1	0.11
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD12	1	0.11
(1,2426)	1:84:A:SER:HB2	1:86:A:ILE:HD13	1	0.11
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD11	1	0.11
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD12	1	0.11
(1,2426)	1:84:A:SER:HB3	1:86:A:ILE:HD13	1	0.11
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE2	20	0.11
(1,2402)	1:77:A:ILE:HD11	1:87:A:LYS:HE3	20	0.11
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE2	20	0.11
(1,2402)	1:77:A:ILE:HD12	1:87:A:LYS:HE3	20	0.11
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE2	20	0.11
(1,2402)	1:77:A:ILE:HD13	1:87:A:LYS:HE3	20	0.11
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE2	18	0.11
(1,2401)	1:77:A:ILE:HG13	1:87:A:LYS:HE3	18	0.11
(1,2389)	1:76:A:VAL:HG11	1:79:A:GLY:H	19	0.11
(1,2389)	1:76:A:VAL:HG12	1:79:A:GLY:H	19	0.11
(1,2389)	1:76:A:VAL:HG13	1:79:A:GLY:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2389)	1:76:A:VAL:HG21	1:79:A:GLY:H	19	0.11
(1,2389)	1:76:A:VAL:HG22	1:79:A:GLY:H	19	0.11
(1,2389)	1:76:A:VAL:HG23	1:79:A:GLY:H	19	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG11	17	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG12	17	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG13	17	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG21	17	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG22	17	0.11
(1,2330)	1:68:A:ASP:HB2	1:74:A:VAL:HG23	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG11	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG12	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG13	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG21	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG22	17	0.11
(1,2330)	1:68:A:ASP:HB3	1:74:A:VAL:HG23	17	0.11
(1,2329)	1:68:A:ASP:HB2	1:74:A:VAL:HB	12	0.11
(1,2329)	1:68:A:ASP:HB3	1:74:A:VAL:HB	12	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG11	3	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG12	3	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG13	3	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG21	3	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG22	3	0.11
(1,2325)	1:68:A:ASP:HA	1:74:A:VAL:HG23	3	0.11
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB2	2	0.11
(1,2272)	1:61:A:LYS:HD2	1:62:A:SER:HB3	2	0.11
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB2	2	0.11
(1,2272)	1:61:A:LYS:HD3	1:62:A:SER:HB3	2	0.11
(1,2250)	1:60:A:ARG:HD2	1:81:A:GLN:HE22	18	0.11
(1,2250)	1:60:A:ARG:HD3	1:81:A:GLN:HE22	18	0.11
(1,2242)	1:60:A:ARG:HG2	1:81:A:GLN:HE21	2	0.11
(1,2242)	1:60:A:ARG:HG3	1:81:A:GLN:HE21	2	0.11
(1,2242)	1:60:A:ARG:HG2	1:81:A:GLN:HE21	10	0.11
(1,2242)	1:60:A:ARG:HG3	1:81:A:GLN:HE21	10	0.11
(1,2221)	1:57:A:ARG:HG2	1:58:A:CYS:H	11	0.11
(1,2221)	1:57:A:ARG:HG3	1:58:A:CYS:H	11	0.11
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	9	0.11
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	9	0.11
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD2	15	0.11
(1,2216)	1:56:A:ASP:H	1:57:A:ARG:HD3	15	0.11
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB2	16	0.11
(1,2212)	1:55:A:LYS:HE2	1:56:A:ASP:HB3	16	0.11
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:55:A:LYS:HE3	1:56:A:ASP:HB3	16	0.11
(1,2196)	1:55:A:LYS:H	1:55:A:LYS:HG2	9	0.11
(1,2196)	1:55:A:LYS:H	1:55:A:LYS:HG3	9	0.11
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD2	4	0.11
(1,2194)	1:54:A:ALA:HB1	1:57:A:ARG:HD3	4	0.11
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD2	4	0.11
(1,2194)	1:54:A:ALA:HB2	1:57:A:ARG:HD3	4	0.11
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD2	4	0.11
(1,2194)	1:54:A:ALA:HB3	1:57:A:ARG:HD3	4	0.11
(1,2161)	1:47:A:LYS:HB2	1:52:A:THR:HA	8	0.11
(1,2161)	1:47:A:LYS:HB3	1:52:A:THR:HA	8	0.11
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE2	8	0.11
(1,2158)	1:47:A:LYS:HA	1:47:A:LYS:HE3	8	0.11
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	3	0.11
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	3	0.11
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	3	0.11
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	3	0.11
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	3	0.11
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	3	0.11
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA2	11	0.11
(1,2137)	1:43:A:ILE:HG21	1:53:A:GLY:HA3	11	0.11
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA2	11	0.11
(1,2137)	1:43:A:ILE:HG22	1:53:A:GLY:HA3	11	0.11
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA2	11	0.11
(1,2137)	1:43:A:ILE:HG23	1:53:A:GLY:HA3	11	0.11
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD2	8	0.11
(1,2124)	1:38:A:GLY:HA3	1:59:A:ARG:HD3	8	0.11
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	8	0.11
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	8	0.11
(1,2117)	1:37:A:SER:HB2	1:58:A:CYS:HA	9	0.11
(1,2117)	1:37:A:SER:HB3	1:58:A:CYS:HA	9	0.11
(1,2107)	1:35:A:GLY:HA2	1:106:A:ILE:HG21	13	0.11
(1,2107)	1:35:A:GLY:HA2	1:106:A:ILE:HG22	13	0.11
(1,2107)	1:35:A:GLY:HA2	1:106:A:ILE:HG23	13	0.11
(1,2107)	1:35:A:GLY:HA3	1:106:A:ILE:HG21	13	0.11
(1,2107)	1:35:A:GLY:HA3	1:106:A:ILE:HG22	13	0.11
(1,2107)	1:35:A:GLY:HA3	1:106:A:ILE:HG23	13	0.11
(1,2092)	1:28:A:LEU:HD11	1:29:A:ASN:H	15	0.11
(1,2092)	1:28:A:LEU:HD12	1:29:A:ASN:H	15	0.11
(1,2092)	1:28:A:LEU:HD13	1:29:A:ASN:H	15	0.11
(1,2092)	1:28:A:LEU:HD21	1:29:A:ASN:H	15	0.11
(1,2092)	1:28:A:LEU:HD22	1:29:A:ASN:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2092)	1:28:A:LEU:HD23	1:29:A:ASN:H	15	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	1	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	1	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD11	3	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD12	3	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD13	3	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD21	3	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD22	3	0.11
(1,2088)	1:27:A:TYR:HE1	1:46:A:LEU:HD23	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD11	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD12	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD13	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD21	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD22	3	0.11
(1,2088)	1:27:A:TYR:HE2	1:46:A:LEU:HD23	3	0.11
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG2	11	0.11
(1,2071)	1:20:A:PHE:HD1	1:21:A:GLU:HG3	11	0.11
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG2	11	0.11
(1,2071)	1:20:A:PHE:HD2	1:21:A:GLU:HG3	11	0.11
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB2	2	0.11
(1,2066)	1:18:A:ASP:H	1:18:A:ASP:HB3	2	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	6	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	6	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	6	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD21	6	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD22	6	0.11
(1,2046)	1:15:A:GLN:HB2	1:28:A:LEU:HD23	6	0.11
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD2	1	0.11
(1,2033)	1:8:A:LEU:HD11	1:57:A:ARG:HD3	1	0.11
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD2	1	0.11
(1,2033)	1:8:A:LEU:HD12	1:57:A:ARG:HD3	1	0.11
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2033)	1:8:A:LEU:HD13	1:57:A:ARG:HD3	1	0.11
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD2	1	0.11
(1,2033)	1:8:A:LEU:HD21	1:57:A:ARG:HD3	1	0.11
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD2	1	0.11
(1,2033)	1:8:A:LEU:HD22	1:57:A:ARG:HD3	1	0.11
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD2	1	0.11
(1,2033)	1:8:A:LEU:HD23	1:57:A:ARG:HD3	1	0.11
(1,2016)	1:8:A:LEU:HD11	1:10:A:PHE:H	18	0.11
(1,2016)	1:8:A:LEU:HD12	1:10:A:PHE:H	18	0.11
(1,2016)	1:8:A:LEU:HD13	1:10:A:PHE:H	18	0.11
(1,2016)	1:8:A:LEU:HD21	1:10:A:PHE:H	18	0.11
(1,2016)	1:8:A:LEU:HD22	1:10:A:PHE:H	18	0.11
(1,2016)	1:8:A:LEU:HD23	1:10:A:PHE:H	18	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD11	2	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD12	2	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD13	2	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD21	2	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD22	2	0.11
(1,1990)	1:4:A:ALA:HB1	1:28:A:LEU:HD23	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD11	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD12	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD13	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD21	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD22	2	0.11
(1,1990)	1:4:A:ALA:HB2	1:28:A:LEU:HD23	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD11	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD12	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD13	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD21	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD22	2	0.11
(1,1990)	1:4:A:ALA:HB3	1:28:A:LEU:HD23	2	0.11
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB2	12	0.11
(1,1982)	1:1:A:GLN:HE22	1:21:A:GLU:HB3	12	0.11
(1,1952)	1:36:A:TYR:HE1	1:61:A:LYS:H	16	0.11
(1,1952)	1:36:A:TYR:HE2	1:61:A:LYS:H	16	0.11
(1,1950)	1:36:A:TYR:HE1	1:60:A:ARG:HA	11	0.11
(1,1950)	1:36:A:TYR:HE2	1:60:A:ARG:HA	11	0.11
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE1	13	0.11
(1,1949)	1:10:A:PHE:HA	1:36:A:TYR:HE2	13	0.11
(1,1947)	1:36:A:TYR:HE1	1:59:A:ARG:HA	1	0.11
(1,1947)	1:36:A:TYR:HE2	1:59:A:ARG:HA	1	0.11
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	9	0.11
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	9	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	9	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	9	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	9	0.11
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG21	16	0.11
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG22	16	0.11
(1,1942)	1:27:A:TYR:HD1	1:44:A:ILE:HG23	16	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG21	16	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG22	16	0.11
(1,1942)	1:27:A:TYR:HD2	1:44:A:ILE:HG23	16	0.11
(1,1925)	1:8:A:LEU:HD21	1:9:A:PRO:HG2	10	0.11
(1,1925)	1:8:A:LEU:HD22	1:9:A:PRO:HG2	10	0.11
(1,1925)	1:8:A:LEU:HD23	1:9:A:PRO:HG2	10	0.11
(1,1902)	1:24:A:ILE:HA	1:49:A:SER:HA	3	0.11
(1,1902)	1:24:A:ILE:HA	1:49:A:SER:HA	11	0.11
(1,1880)	1:44:A:ILE:HB	1:46:A:LEU:HD11	8	0.11
(1,1880)	1:44:A:ILE:HB	1:46:A:LEU:HD12	8	0.11
(1,1880)	1:44:A:ILE:HB	1:46:A:LEU:HD13	8	0.11
(1,1876)	1:45:A:CYS:HA	1:46:A:LEU:HG	18	0.11
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE1	4	0.11
(1,1864)	1:8:A:LEU:HD21	1:10:A:PHE:HE2	4	0.11
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE1	4	0.11
(1,1864)	1:8:A:LEU:HD22	1:10:A:PHE:HE2	4	0.11
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE1	4	0.11
(1,1864)	1:8:A:LEU:HD23	1:10:A:PHE:HE2	4	0.11
(1,1861)	1:14:A:THR:HB	1:29:A:ASN:HB3	20	0.11
(1,1803)	1:43:A:ILE:HG21	1:54:A:ALA:HA	20	0.11
(1,1803)	1:43:A:ILE:HG22	1:54:A:ALA:HA	20	0.11
(1,1803)	1:43:A:ILE:HG23	1:54:A:ALA:HA	20	0.11
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG21	7	0.11
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG22	7	0.11
(1,1793)	1:82:A:PHE:HB2	1:111:A:VAL:HG23	7	0.11
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	11	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	1	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	1	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	1	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG21	12	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG22	12	0.11
(1,1782)	1:27:A:TYR:HB2	1:44:A:ILE:HG23	12	0.11
(1,1770)	1:38:A:GLY:HA3	1:39:A:ARG:HA	11	0.11
(1,1761)	1:74:A:VAL:HG11	1:88:A:TYR:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1761)	1:74:A:VAL:HG12	1:88:A:TYR:HA	5	0.11
(1,1761)	1:74:A:VAL:HG13	1:88:A:TYR:HA	5	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	4	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	4	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	4	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD21	16	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD22	16	0.11
(1,1748)	1:44:A:ILE:HB	1:46:A:LEU:HD23	16	0.11
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD11	17	0.11
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD12	17	0.11
(1,1747)	1:15:A:GLN:HB2	1:28:A:LEU:HD13	17	0.11
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	6	0.11
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	6	0.11
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE1	14	0.11
(1,1746)	1:9:A:PRO:HG3	1:10:A:PHE:HE2	14	0.11
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD11	10	0.11
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD12	10	0.11
(1,1743)	1:82:A:PHE:HE1	1:106:A:ILE:HD13	10	0.11
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD11	10	0.11
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD12	10	0.11
(1,1743)	1:82:A:PHE:HE2	1:106:A:ILE:HD13	10	0.11
(1,1730)	1:85:A:GLN:HB2	1:113:A:TRP:HZ3	8	0.11
(1,1723)	1:24:A:ILE:HG13	1:46:A:LEU:HA	2	0.11
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB1	9	0.11
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB2	9	0.11
(1,1721)	1:30:A:TYR:HE1	1:54:A:ALA:HB3	9	0.11
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB1	9	0.11
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB2	9	0.11
(1,1721)	1:30:A:TYR:HE2	1:54:A:ALA:HB3	9	0.11
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB1	14	0.11
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB2	14	0.11
(1,1720)	1:44:A:ILE:H	1:54:A:ALA:HB3	14	0.11
(1,1689)	1:38:A:GLY:HA2	1:58:A:CYS:HA	20	0.11
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	2	0.11
(1,1686)	1:58:A:CYS:HA	1:59:A:ARG:HD2	6	0.11
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	1	0.11
(1,1676)	1:25:A:GLY:HA2	1:44:A:ILE:HB	18	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	6	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	6	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	6	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	11	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	11	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	12	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	12	0.11
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	12	0.11
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	13	0.11
(1,1633)	1:77:A:ILE:HG13	1:85:A:GLN:HG2	14	0.11
(1,1628)	1:15:A:GLN:HG2	1:29:A:ASN:HB3	13	0.11
(1,1628)	1:15:A:GLN:HG3	1:29:A:ASN:HB3	13	0.11
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	1	0.11
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	1	0.11
(1,1560)	1:5:A:PRO:HB2	1:6:A:GLU:HA	16	0.11
(1,1556)	1:40:A:PRO:HG2	1:41:A:PHE:HA	14	0.11
(1,1556)	1:40:A:PRO:HG3	1:41:A:PHE:HA	14	0.11
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	5	0.11
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	5	0.11
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	5	0.11
(1,1552)	1:96:A:LEU:HD21	1:97:A:ILE:H	11	0.11
(1,1552)	1:96:A:LEU:HD22	1:97:A:ILE:H	11	0.11
(1,1552)	1:96:A:LEU:HD23	1:97:A:ILE:H	11	0.11
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD11	16	0.11
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD12	16	0.11
(1,1549)	1:117:A:THR:H	1:119:A:ILE:HD13	16	0.11
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	11	0.11
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	11	0.11
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	11	0.11
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	16	0.11
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	16	0.11
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	16	0.11
(1,1543)	1:94:A:TYR:HA	1:122:A:ARG:HA	3	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD11	19	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD12	19	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD13	19	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD11	20	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD12	20	0.11
(1,1531)	1:103:A:THR:HB	1:105:A:ILE:HD13	20	0.11
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	2	0.11
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	2	0.11
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	2	0.11
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	2	0.11
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	2	0.11
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	2	0.11
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD1	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:91:A:THR:HG21	1:94:A:TYR:HD2	18	0.11
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD1	18	0.11
(1,1522)	1:91:A:THR:HG22	1:94:A:TYR:HD2	18	0.11
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD1	18	0.11
(1,1522)	1:91:A:THR:HG23	1:94:A:TYR:HD2	18	0.11
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	18	0.11
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	18	0.11
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	18	0.11
(1,1519)	1:91:A:THR:HG21	1:94:A:TYR:HB2	19	0.11
(1,1519)	1:91:A:THR:HG22	1:94:A:TYR:HB2	19	0.11
(1,1519)	1:91:A:THR:HG23	1:94:A:TYR:HB2	19	0.11
(1,1487)	1:44:A:ILE:HD11	1:52:A:THR:HB	3	0.11
(1,1487)	1:44:A:ILE:HD12	1:52:A:THR:HB	3	0.11
(1,1487)	1:44:A:ILE:HD13	1:52:A:THR:HB	3	0.11
(1,1461)	1:4:A:ALA:H	1:20:A:PHE:HA	4	0.11
(1,1453)	1:63:A:CYS:HA	1:64:A:ARG:HB3	12	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	7	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	7	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	7	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD11	18	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD12	18	0.11
(1,1445)	1:85:A:GLN:HA	1:86:A:ILE:HD13	18	0.11
(1,1439)	1:44:A:ILE:HD11	1:51:A:TRP:HA	16	0.11
(1,1439)	1:44:A:ILE:HD12	1:51:A:TRP:HA	16	0.11
(1,1439)	1:44:A:ILE:HD13	1:51:A:TRP:HA	16	0.11
(1,1414)	1:63:A:CYS:HA	1:111:A:VAL:HG21	18	0.11
(1,1414)	1:63:A:CYS:HA	1:111:A:VAL:HG22	18	0.11
(1,1414)	1:63:A:CYS:HA	1:111:A:VAL:HG23	18	0.11
(1,1390)	1:87:A:LYS:HB3	1:88:A:TYR:HD1	13	0.11
(1,1390)	1:87:A:LYS:HB3	1:88:A:TYR:HD2	13	0.11
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	8	0.11
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	8	0.11
(1,1340)	1:38:A:GLY:HA2	1:39:A:ARG:HB3	15	0.11
(1,1340)	1:38:A:GLY:HA2	1:39:A:ARG:HB3	17	0.11
(1,1306)	1:65:A:ASN:HA	1:67:A:PRO:HG3	13	0.11
(1,1287)	1:77:A:ILE:HD11	1:78:A:LYS:H	14	0.11
(1,1287)	1:77:A:ILE:HD12	1:78:A:LYS:H	14	0.11
(1,1287)	1:77:A:ILE:HD13	1:78:A:LYS:H	14	0.11
(1,1272)	1:14:A:THR:HG21	1:29:A:ASN:HB2	16	0.11
(1,1272)	1:14:A:THR:HG22	1:29:A:ASN:HB2	16	0.11
(1,1272)	1:14:A:THR:HG23	1:29:A:ASN:HB2	16	0.11
(1,1272)	1:14:A:THR:HG21	1:29:A:ASN:HB2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:14:A:THR:HG22	1:29:A:ASN:HB2	18	0.11
(1,1272)	1:14:A:THR:HG23	1:29:A:ASN:HB2	18	0.11
(1,1269)	1:14:A:THR:HG21	1:29:A:ASN:H	7	0.11
(1,1269)	1:14:A:THR:HG22	1:29:A:ASN:H	7	0.11
(1,1269)	1:14:A:THR:HG23	1:29:A:ASN:H	7	0.11
(1,1240)	1:4:A:ALA:HB1	1:51:A:TRP:HZ2	1	0.11
(1,1240)	1:4:A:ALA:HB2	1:51:A:TRP:HZ2	1	0.11
(1,1240)	1:4:A:ALA:HB3	1:51:A:TRP:HZ2	1	0.11
(1,1227)	1:64:A:ARG:HA	1:113:A:TRP:HZ2	11	0.11
(1,1196)	1:97:A:ILE:HD11	1:121:A:ASP:HB3	6	0.11
(1,1196)	1:97:A:ILE:HD12	1:121:A:ASP:HB3	6	0.11
(1,1196)	1:97:A:ILE:HD13	1:121:A:ASP:HB3	6	0.11
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG21	13	0.11
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG22	13	0.11
(1,1170)	1:65:A:ASN:HD21	1:80:A:ILE:HG23	13	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG21	19	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG22	19	0.11
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG23	19	0.11
(1,1112)	1:33:A:ARG:H	1:36:A:TYR:HB3	14	0.11
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD1	19	0.11
(1,1085)	1:9:A:PRO:HG3	1:10:A:PHE:HD2	19	0.11
(1,1040)	1:95:A:ARG:HB2	1:121:A:ASP:HB3	15	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	3	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	3	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	3	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	3	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	3	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	3	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	3	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	3	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	3	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD11	15	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD12	15	0.11
(1,1030)	1:105:A:ILE:HD11	1:106:A:ILE:HD13	15	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD11	15	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD12	15	0.11
(1,1030)	1:105:A:ILE:HD12	1:106:A:ILE:HD13	15	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD11	15	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD12	15	0.11
(1,1030)	1:105:A:ILE:HD13	1:106:A:ILE:HD13	15	0.11
(1,1014)	1:105:A:ILE:HB	1:106:A:ILE:HD11	8	0.11
(1,1014)	1:105:A:ILE:HB	1:106:A:ILE:HD12	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:105:A:ILE:HB	1:106:A:ILE:HD13	8	0.11
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG11	20	0.11
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG12	20	0.11
(1,986)	1:81:A:GLN:HE21	1:111:A:VAL:HG13	20	0.11
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	1	0.11
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	1	0.11
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	1	0.11
(1,954)	1:68:A:ASP:H	1:69:A:PRO:HA	17	0.11
(1,952)	1:107:A:SER:H	1:110:A:THR:H	8	0.11
(1,952)	1:107:A:SER:H	1:110:A:THR:H	10	0.11
(1,939)	1:81:A:GLN:HB2	1:81:A:GLN:HE21	20	0.11
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	6	0.11
(1,937)	1:81:A:GLN:HE22	1:82:A:PHE:HB3	6	0.11
(1,926)	1:65:A:ASN:HA	1:65:A:ASN:HD21	13	0.11
(1,914)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	9	0.11
(1,892)	1:3:A:ASN:HD21	1:4:A:ALA:H	2	0.11
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	18	0.11
(1,882)	1:4:A:ALA:H	1:51:A:TRP:HE1	19	0.11
(1,870)	1:88:A:TYR:HD1	1:101:A:SER:H	12	0.11
(1,870)	1:88:A:TYR:HD2	1:101:A:SER:H	12	0.11
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	1	0.11
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	7	0.11
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	11	0.11
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	17	0.11
(1,808)	1:4:A:ALA:HA	1:20:A:PHE:H	2	0.11
(1,807)	1:20:A:PHE:H	1:21:A:GLU:H	10	0.11
(1,802)	1:19:A:GLU:H	1:20:A:PHE:HB2	2	0.11
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD1	10	0.11
(1,776)	1:17:A:THR:H	1:20:A:PHE:HD2	10	0.11
(1,747)	1:24:A:ILE:H	1:24:A:ILE:HG12	5	0.11
(1,725)	1:52:A:THR:HG21	1:53:A:GLY:H	17	0.11
(1,725)	1:52:A:THR:HG22	1:53:A:GLY:H	17	0.11
(1,725)	1:52:A:THR:HG23	1:53:A:GLY:H	17	0.11
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD1	7	0.11
(1,693)	1:61:A:LYS:H	1:82:A:PHE:HD2	7	0.11
(1,689)	1:61:A:LYS:HB2	1:62:A:SER:H	16	0.11
(1,652)	1:69:A:PRO:HB3	1:74:A:VAL:H	12	0.11
(1,628)	1:77:A:ILE:H	1:86:A:ILE:HB	8	0.11
(1,626)	1:75:A:HIS:HB3	1:77:A:ILE:H	13	0.11
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	2	0.11
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	2	0.11
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG21	10	0.11
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG22	10	0.11
(1,621)	1:44:A:ILE:H	1:52:A:THR:HG23	10	0.11
(1,591)	1:84:A:SER:H	1:104:A:CYS:H	1	0.11
(1,591)	1:84:A:SER:H	1:104:A:CYS:H	10	0.11
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	7	0.11
(1,565)	1:74:A:VAL:HB	1:87:A:LYS:H	16	0.11
(1,565)	1:74:A:VAL:HB	1:87:A:LYS:H	17	0.11
(1,562)	1:75:A:HIS:HB3	1:87:A:LYS:H	6	0.11
(1,497)	1:94:A:TYR:HB2	1:96:A:LEU:H	6	0.11
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD11	11	0.11
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD12	11	0.11
(1,458)	1:83:A:GLY:H	1:105:A:ILE:HD13	11	0.11
(1,447)	1:106:A:ILE:HG21	1:108:A:GLY:H	4	0.11
(1,447)	1:106:A:ILE:HG22	1:108:A:GLY:H	4	0.11
(1,447)	1:106:A:ILE:HG23	1:108:A:GLY:H	4	0.11
(1,437)	1:106:A:ILE:HB	1:107:A:SER:H	10	0.11
(1,407)	1:113:A:TRP:HB2	1:115:A:GLN:H	15	0.11
(1,405)	1:103:A:THR:HB	1:115:A:GLN:H	20	0.11
(1,404)	1:99:A:SER:HB2	1:115:A:GLN:H	15	0.11
(1,380)	1:119:A:ILE:HB	1:120:A:CYS:H	5	0.11
(1,377)	1:94:A:TYR:HE1	1:120:A:CYS:H	2	0.11
(1,377)	1:94:A:TYR:HE2	1:120:A:CYS:H	2	0.11
(1,370)	1:30:A:TYR:H	1:42:A:SER:HB3	6	0.11
(1,367)	1:30:A:TYR:H	1:42:A:SER:HA	12	0.11
(1,314)	1:85:A:GLN:HG3	1:102:A:ALA:H	5	0.11
(1,290)	1:86:A:ILE:HD11	1:104:A:CYS:H	19	0.11
(1,290)	1:86:A:ILE:HD12	1:104:A:CYS:H	19	0.11
(1,290)	1:86:A:ILE:HD13	1:104:A:CYS:H	19	0.11
(1,261)	1:54:A:ALA:H	1:55:A:LYS:H	18	0.11
(1,254)	1:14:A:THR:HA	1:15:A:GLN:H	1	0.11
(1,215)	1:43:A:ILE:H	1:51:A:TRP:HE3	16	0.11
(1,186)	1:88:A:TYR:HB3	1:119:A:ILE:H	18	0.11
(1,181)	1:10:A:PHE:HE1	1:58:A:CYS:H	11	0.11
(1,181)	1:10:A:PHE:HE2	1:58:A:CYS:H	11	0.11
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	13	0.11
(1,150)	1:92:A:LYS:HB2	1:93:A:GLY:H	9	0.11
(1,141)	1:88:A:TYR:H	1:89:A:SER:H	7	0.11
(1,141)	1:88:A:TYR:H	1:89:A:SER:H	10	0.11
(1,140)	1:80:A:ILE:H	1:85:A:GLN:H	13	0.11
(1,136)	1:76:A:VAL:HA	1:80:A:ILE:H	10	0.11
(1,123)	1:8:A:LEU:HD21	1:10:A:PHE:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:8:A:LEU:HD22	1:10:A:PHE:H	18	0.11
(1,123)	1:8:A:LEU:HD23	1:10:A:PHE:H	18	0.11
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	1	0.11
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	6	0.11
(1,89)	1:97:A:ILE:H	1:119:A:ILE:HB	15	0.11
(1,86)	1:37:A:SER:H	1:60:A:ARG:H	1	0.11
(1,80)	1:60:A:ARG:H	1:82:A:PHE:HB3	2	0.11
(1,51)	1:86:A:ILE:H	1:103:A:THR:HG21	2	0.11
(1,51)	1:86:A:ILE:H	1:103:A:THR:HG22	2	0.11
(1,51)	1:86:A:ILE:H	1:103:A:THR:HG23	2	0.11
(1,45)	1:12:A:ARG:H	1:13:A:PRO:HD2	17	0.11
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	8	0.11
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	9	0.11
(1,8)	1:91:A:THR:HG21	1:95:A:ARG:H	12	0.11
(1,8)	1:91:A:THR:HG22	1:95:A:ARG:H	12	0.11
(1,8)	1:91:A:THR:HG23	1:95:A:ARG:H	12	0.11
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	9	0.1
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	9	0.1
(1,2565)	1:115:A:GLN:HG2	1:116:A:GLU:H	17	0.1
(1,2565)	1:115:A:GLN:HG3	1:116:A:GLU:H	17	0.1
(1,2507)	1:96:A:LEU:HD11	1:100:A:SER:HA	5	0.1
(1,2507)	1:96:A:LEU:HD12	1:100:A:SER:HA	5	0.1
(1,2507)	1:96:A:LEU:HD13	1:100:A:SER:HA	5	0.1
(1,2507)	1:96:A:LEU:HD21	1:100:A:SER:HA	5	0.1
(1,2507)	1:96:A:LEU:HD22	1:100:A:SER:HA	5	0.1
(1,2507)	1:96:A:LEU:HD23	1:100:A:SER:HA	5	0.1
(1,2487)	1:94:A:TYR:HE1	1:120:A:CYS:HB2	6	0.1
(1,2487)	1:94:A:TYR:HE1	1:120:A:CYS:HB3	6	0.1
(1,2487)	1:94:A:TYR:HE2	1:120:A:CYS:HB2	6	0.1
(1,2487)	1:94:A:TYR:HE2	1:120:A:CYS:HB3	6	0.1
(1,2480)	1:92:A:LYS:HD2	1:94:A:TYR:H	16	0.1
(1,2480)	1:92:A:LYS:HD3	1:94:A:TYR:H	16	0.1
(1,2465)	1:90:A:CYS:HB2	1:120:A:CYS:HA	14	0.1
(1,2465)	1:90:A:CYS:HB3	1:120:A:CYS:HA	14	0.1
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE1	18	0.1
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE2	18	0.1
(1,2353)	1:71:A:ASN:HB2	1:73:A:MET:HE3	18	0.1
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE1	18	0.1
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE2	18	0.1
(1,2353)	1:71:A:ASN:HB3	1:73:A:MET:HE3	18	0.1
(1,2154)	1:46:A:LEU:HD11	1:52:A:THR:HB	16	0.1
(1,2154)	1:46:A:LEU:HD12	1:52:A:THR:HB	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2154)	1:46:A:LEU:HD13	1:52:A:THR:HB	16	0.1
(1,2154)	1:46:A:LEU:HD21	1:52:A:THR:HB	16	0.1
(1,2154)	1:46:A:LEU:HD22	1:52:A:THR:HB	16	0.1
(1,2154)	1:46:A:LEU:HD23	1:52:A:THR:HB	16	0.1
(1,2134)	1:41:A:PHE:HB2	1:42:A:SER:H	3	0.1
(1,2134)	1:41:A:PHE:HB3	1:42:A:SER:H	3	0.1
(1,1948)	1:25:A:GLY:HA2	1:27:A:TYR:HE1	10	0.1
(1,1948)	1:25:A:GLY:HA2	1:27:A:TYR:HE2	10	0.1
(1,1925)	1:8:A:LEU:HD21	1:9:A:PRO:HG2	3	0.1
(1,1925)	1:8:A:LEU:HD22	1:9:A:PRO:HG2	3	0.1
(1,1925)	1:8:A:LEU:HD23	1:9:A:PRO:HG2	3	0.1
(1,1899)	1:46:A:LEU:HG	1:52:A:THR:HB	3	0.1
(1,1841)	1:85:A:GLN:HG3	1:101:A:SER:HA	18	0.1
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD11	11	0.1
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD12	11	0.1
(1,1837)	1:85:A:GLN:HG3	1:86:A:ILE:HD13	11	0.1
(1,1827)	1:87:A:LYS:HG3	1:101:A:SER:HA	2	0.1
(1,1789)	1:16:A:LEU:HG	1:17:A:THR:HA	16	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	4	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	4	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	4	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG21	14	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG22	14	0.1
(1,1780)	1:26:A:THR:HB	1:44:A:ILE:HG23	14	0.1
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	3	0.1
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	3	0.1
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	3	0.1
(1,1742)	1:106:A:ILE:HD11	1:112:A:ILE:H	18	0.1
(1,1742)	1:106:A:ILE:HD12	1:112:A:ILE:H	18	0.1
(1,1742)	1:106:A:ILE:HD13	1:112:A:ILE:H	18	0.1
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG21	19	0.1
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG22	19	0.1
(1,1717)	1:110:A:THR:HG21	1:112:A:ILE:HG23	19	0.1
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG21	19	0.1
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG22	19	0.1
(1,1717)	1:110:A:THR:HG22	1:112:A:ILE:HG23	19	0.1
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG21	19	0.1
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG22	19	0.1
(1,1717)	1:110:A:THR:HG23	1:112:A:ILE:HG23	19	0.1
(1,1700)	1:5:A:PRO:HD2	1:20:A:PHE:HB3	19	0.1
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE1	12	0.1
(1,1698)	1:18:A:ASP:HA	1:20:A:PHE:HE2	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB1	18	0.1
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB2	18	0.1
(1,1669)	1:10:A:PHE:HD1	1:11:A:ALA:HB3	18	0.1
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB1	18	0.1
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB2	18	0.1
(1,1669)	1:10:A:PHE:HD2	1:11:A:ALA:HB3	18	0.1
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG21	4	0.1
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG22	4	0.1
(1,1644)	1:85:A:GLN:HB2	1:103:A:THR:HG23	4	0.1
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	14	0.1
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	14	0.1
(1,1627)	1:15:A:GLN:HG2	1:29:A:ASN:HB2	17	0.1
(1,1627)	1:15:A:GLN:HG3	1:29:A:ASN:HB2	17	0.1
(1,1560)	1:5:A:PRO:HB2	1:6:A:GLU:HA	11	0.1
(1,1546)	1:77:A:ILE:HD11	1:85:A:GLN:HG2	20	0.1
(1,1546)	1:77:A:ILE:HD12	1:85:A:GLN:HG2	20	0.1
(1,1546)	1:77:A:ILE:HD13	1:85:A:GLN:HG2	20	0.1
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD1	8	0.1
(1,1369)	1:5:A:PRO:HD2	1:22:A:PHE:HD2	8	0.1
(1,1346)	1:27:A:TYR:HE1	1:44:A:ILE:HB	19	0.1
(1,1346)	1:27:A:TYR:HE2	1:44:A:ILE:HB	19	0.1
(1,1318)	1:96:A:LEU:HD21	1:100:A:SER:HA	5	0.1
(1,1318)	1:96:A:LEU:HD22	1:100:A:SER:HA	5	0.1
(1,1318)	1:96:A:LEU:HD23	1:100:A:SER:HA	5	0.1
(1,1219)	1:117:A:THR:HG21	1:119:A:ILE:HA	16	0.1
(1,1219)	1:117:A:THR:HG22	1:119:A:ILE:HA	16	0.1
(1,1219)	1:117:A:THR:HG23	1:119:A:ILE:HA	16	0.1
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB2	3	0.1
(1,1198)	1:99:A:SER:HB3	1:115:A:GLN:HB3	3	0.1
(1,1169)	1:80:A:ILE:HB	1:113:A:TRP:HZ2	19	0.1
(1,1164)	1:75:A:HIS:HB3	1:77:A:ILE:HG13	10	0.1
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG21	5	0.1
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG22	5	0.1
(1,1134)	1:51:A:TRP:HA	1:52:A:THR:HG23	5	0.1
(1,1113)	1:31:A:GLU:HA	1:40:A:PRO:HB2	2	0.1
(1,1113)	1:31:A:GLU:HA	1:40:A:PRO:HB3	2	0.1
(1,1033)	1:4:A:ALA:HB1	1:5:A:PRO:HD3	20	0.1
(1,1033)	1:4:A:ALA:HB2	1:5:A:PRO:HD3	20	0.1
(1,1033)	1:4:A:ALA:HB3	1:5:A:PRO:HD3	20	0.1
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD11	16	0.1
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD12	16	0.1
(1,1013)	1:105:A:ILE:HG21	1:106:A:ILE:HD13	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD11	16	0.1
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD12	16	0.1
(1,1013)	1:105:A:ILE:HG22	1:106:A:ILE:HD13	16	0.1
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD11	16	0.1
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD12	16	0.1
(1,1013)	1:105:A:ILE:HG23	1:106:A:ILE:HD13	16	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	6	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	6	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	6	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD21	12	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD22	12	0.1
(1,992)	1:7:A:TRP:HA	1:8:A:LEU:HD23	12	0.1
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG11	20	0.1
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG12	20	0.1
(1,981)	1:61:A:LYS:HE2	1:111:A:VAL:HG13	20	0.1
(1,959)	1:22:A:PHE:H	1:51:A:TRP:HE1	6	0.1
(1,952)	1:107:A:SER:H	1:110:A:THR:H	3	0.1
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	5	0.1
(1,938)	1:81:A:GLN:HB3	1:81:A:GLN:HE21	11	0.1
(1,926)	1:65:A:ASN:HA	1:65:A:ASN:HD21	17	0.1
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG11	7	0.1
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG12	7	0.1
(1,925)	1:81:A:GLN:HE22	1:111:A:VAL:HG13	7	0.1
(1,914)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	7	0.1
(1,911)	1:15:A:GLN:HA	1:15:A:GLN:HE21	20	0.1
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB1	16	0.1
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB2	16	0.1
(1,896)	1:3:A:ASN:HD21	1:4:A:ALA:HB3	16	0.1
(1,890)	1:3:A:ASN:H	1:3:A:ASN:HD21	3	0.1
(1,877)	1:65:A:ASN:HD22	1:113:A:TRP:HE1	10	0.1
(1,866)	1:46:A:LEU:HG	1:47:A:LYS:H	20	0.1
(1,862)	1:13:A:PRO:HA	1:31:A:GLU:H	16	0.1
(1,845)	1:28:A:LEU:HB2	1:29:A:ASN:H	4	0.1
(1,840)	1:29:A:ASN:H	1:30:A:TYR:HE1	20	0.1
(1,840)	1:29:A:ASN:H	1:30:A:TYR:HE2	20	0.1
(1,829)	1:26:A:THR:HA	1:28:A:LEU:H	5	0.1
(1,720)	1:5:A:PRO:HB3	1:6:A:GLU:H	4	0.1
(1,711)	1:43:A:ILE:HA	1:54:A:ALA:H	1	0.1
(1,692)	1:61:A:LYS:H	1:81:A:GLN:HE21	8	0.1
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG21	17	0.1
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG22	17	0.1
(1,690)	1:62:A:SER:H	1:111:A:VAL:HG23	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	4	0.1
(1,680)	1:61:A:LYS:HB3	1:63:A:CYS:H	9	0.1
(1,669)	1:65:A:ASN:H	1:65:A:ASN:HD22	6	0.1
(1,608)	1:82:A:PHE:H	1:111:A:VAL:HG11	6	0.1
(1,608)	1:82:A:PHE:H	1:111:A:VAL:HG12	6	0.1
(1,608)	1:82:A:PHE:H	1:111:A:VAL:HG13	6	0.1
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	1	0.1
(1,580)	1:26:A:THR:H	1:27:A:TYR:H	6	0.1
(1,487)	1:96:A:LEU:HB2	1:100:A:SER:H	3	0.1
(1,483)	1:98:A:GLY:HA2	1:100:A:SER:H	9	0.1
(1,475)	1:99:A:SER:H	1:119:A:ILE:HG12	18	0.1
(1,467)	1:99:A:SER:H	1:116:A:GLU:H	17	0.1
(1,455)	1:83:A:GLY:H	1:111:A:VAL:HB	9	0.1
(1,447)	1:106:A:ILE:HG21	1:108:A:GLY:H	3	0.1
(1,447)	1:106:A:ILE:HG22	1:108:A:GLY:H	3	0.1
(1,447)	1:106:A:ILE:HG23	1:108:A:GLY:H	3	0.1
(1,421)	1:102:A:ALA:HA	1:116:A:GLU:H	2	0.1
(1,376)	1:94:A:TYR:HD1	1:120:A:CYS:H	2	0.1
(1,376)	1:94:A:TYR:HD2	1:120:A:CYS:H	2	0.1
(1,228)	1:111:A:VAL:HG21	1:113:A:TRP:H	3	0.1
(1,228)	1:111:A:VAL:HG22	1:113:A:TRP:H	3	0.1
(1,228)	1:111:A:VAL:HG23	1:113:A:TRP:H	3	0.1
(1,169)	1:14:A:THR:H	1:29:A:ASN:HB2	19	0.1
(1,165)	1:14:A:THR:H	1:15:A:GLN:HA	9	0.1
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE1	3	0.1
(1,163)	1:14:A:THR:H	1:30:A:TYR:HE2	3	0.1
(1,105)	1:46:A:LEU:H	1:49:A:SER:HA	4	0.1
(1,82)	1:36:A:TYR:HA	1:60:A:ARG:H	18	0.1
(1,75)	1:95:A:ARG:H	1:121:A:ASP:H	3	0.1
(1,39)	1:2:A:CYS:H	1:51:A:TRP:HE1	11	0.1
(1,38)	1:2:A:CYS:H	1:51:A:TRP:HZ2	13	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found