Full wwPDB NMR Structure Validation Report (i)

Mar 8, 2026 – 07:55 AM UTC

PDB ID	:	2L29 / pdb_00002l29
BMRB ID	:	17127
Title	:	Complex structure of E4 mutant human IGF2R domain 11 bound to IGF-II
Authors	:	Williams, C.; Hoppe, H.; Rezgui, D.; Strickland, M.; Frago, S.; Ellis, R.Z.; Wattana-Amorn, P.; Prince, S.N.; Zaccheo, O.J.; Forbes, B.; Jones, E.Y.; Crump, M.P.; Hassan, A.B.
Deposited on	:	2010-08-13

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

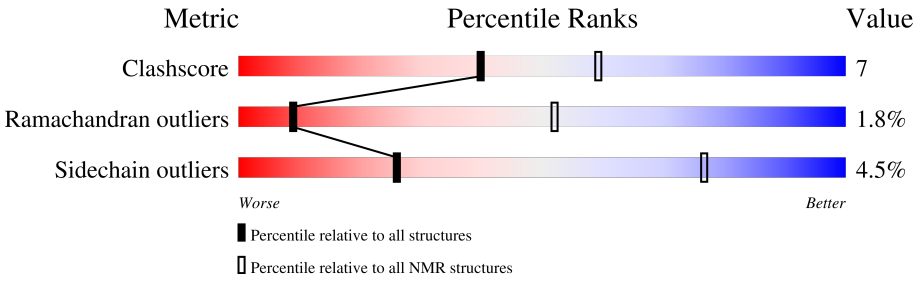
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (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 84%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	142	78% 14% • 6%
2	B	67	51% 7% 42%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:1515-A:1647, B:10-B:28, B:41-B:60 (172)	1.04	10

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 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3146 atoms, of which 1548 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor 2 receptor variant.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2126	672	1049	186	208	11	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1544	LYS	GLU	engineered mutation	UNP Q59EZ3
A	1545	SER	LYS	engineered mutation	UNP Q59EZ3
A	1547	VAL	LEU	engineered mutation	UNP Q59EZ3
A	1648	PRO	-	expression tag	UNP Q59EZ3
A	1649	GLU	-	expression tag	UNP Q59EZ3

- Molecule 2 is a protein called Insulin-like growth factor II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	67	1020	321	499	93	101	6	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

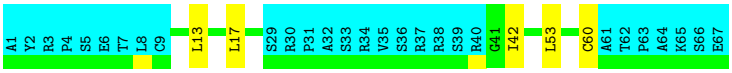
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Insulin-like growth factor 2 receptor variant

Chain A:

• Molecule 2: Insulin-like growth factor II

Chain B:



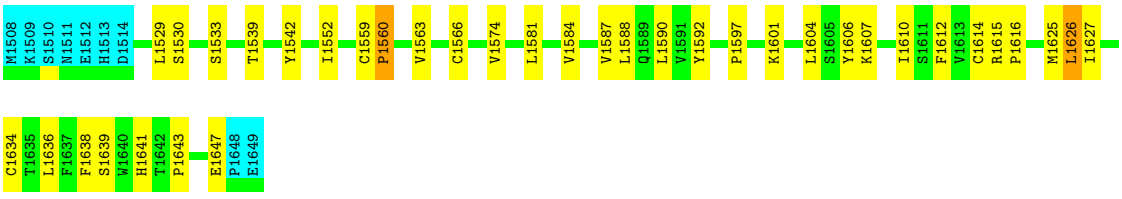
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

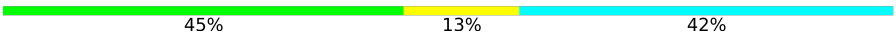
• Molecule 1: Insulin-like growth factor 2 receptor variant

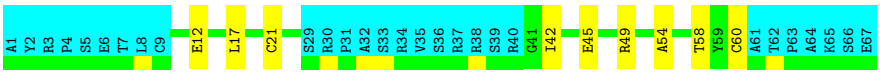
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:

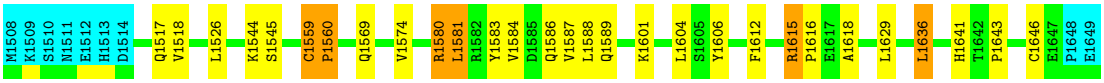




4.2.2 Score per residue for model 2

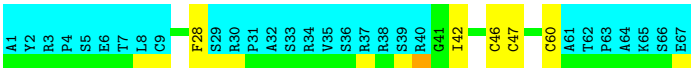
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

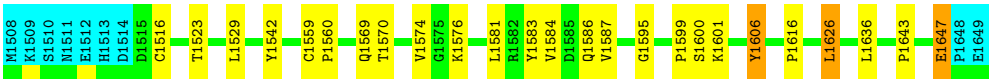
Chain B:



4.2.3 Score per residue for model 3

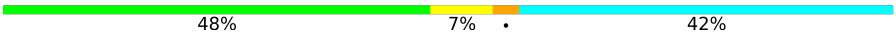
• Molecule 1: Insulin-like growth factor 2 receptor variant

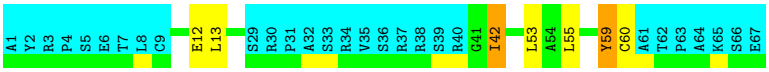
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:

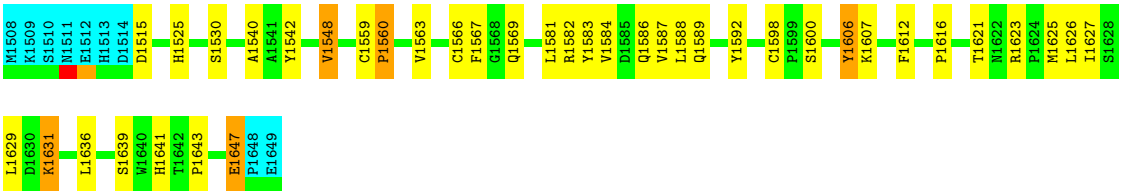




4.2.4 Score per residue for model 4

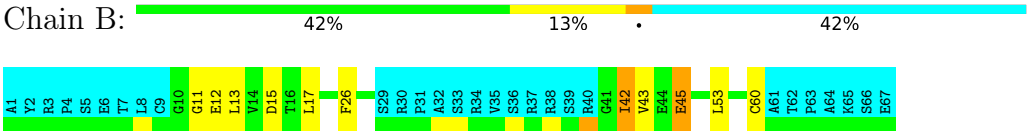
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

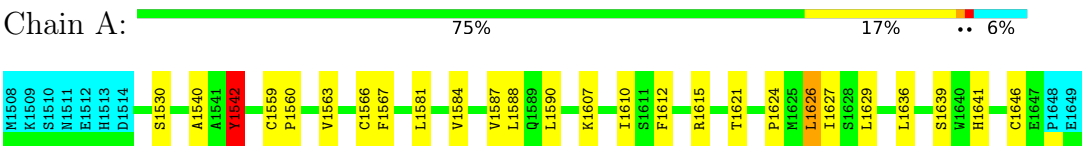
Chain B:



4.2.5 Score per residue for model 5

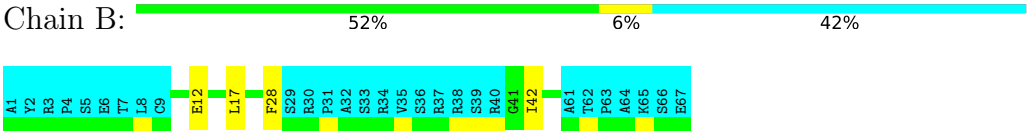
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

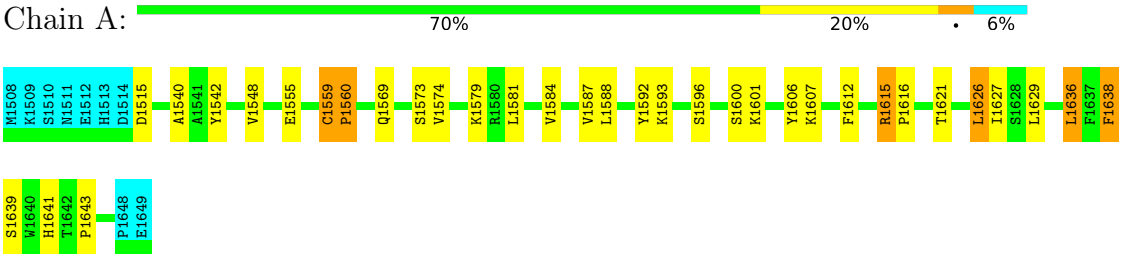
Chain B:



4.2.6 Score per residue for model 6

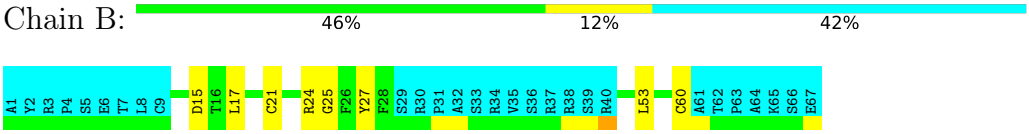
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



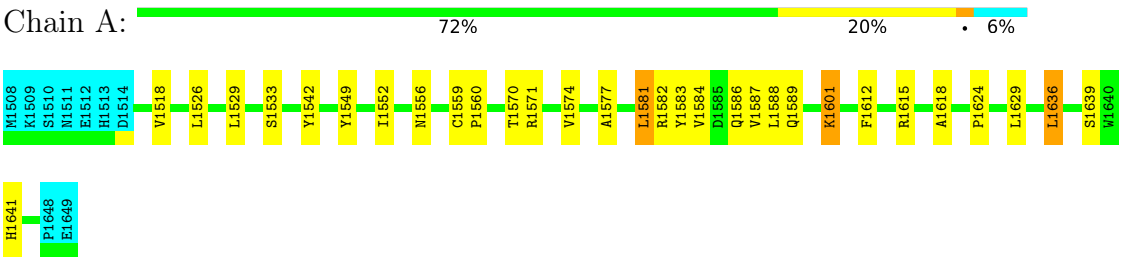
• Molecule 2: Insulin-like growth factor II

Chain B:

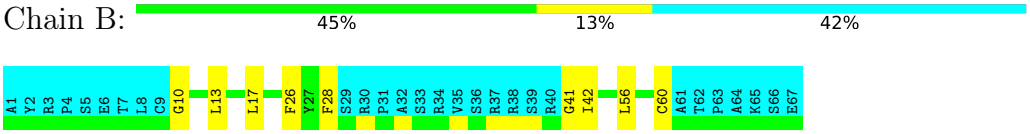


4.2.7 Score per residue for model 7

• Molecule 1: Insulin-like growth factor 2 receptor variant

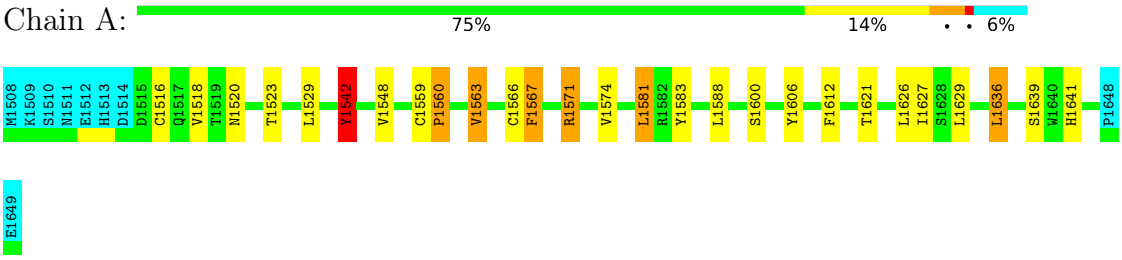


• Molecule 2: Insulin-like growth factor II

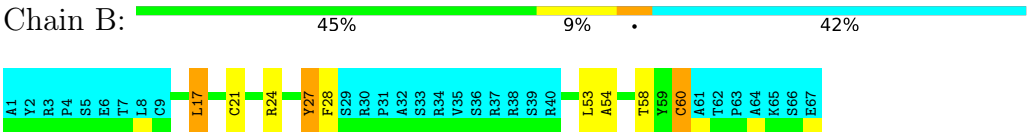


4.2.8 Score per residue for model 8

• Molecule 1: Insulin-like growth factor 2 receptor variant

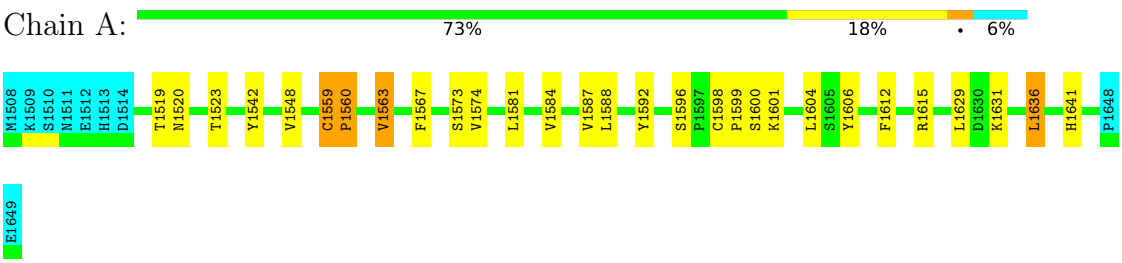


• Molecule 2: Insulin-like growth factor II



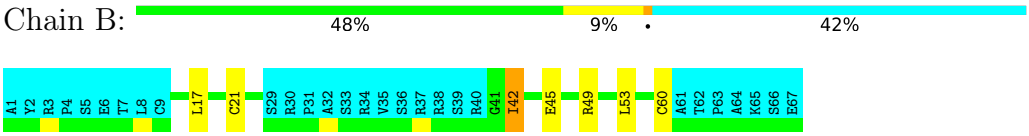
4.2.9 Score per residue for model 9

• Molecule 1: Insulin-like growth factor 2 receptor variant



• Molecule 2: Insulin-like growth factor II

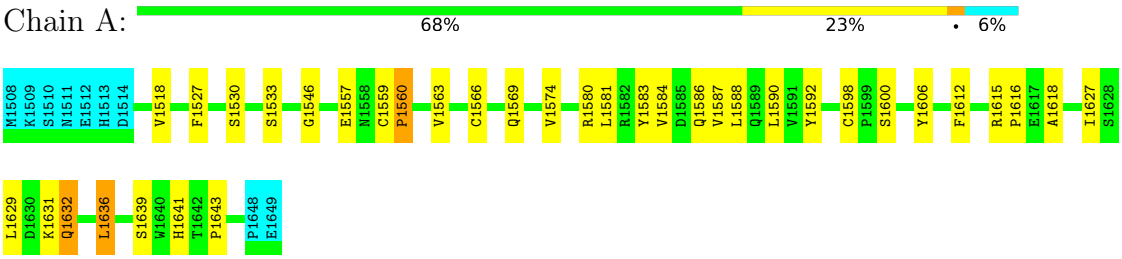
Chain B:



4.2.10 Score per residue for model 10 (medoid)

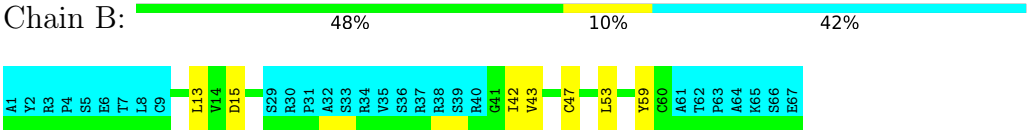
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

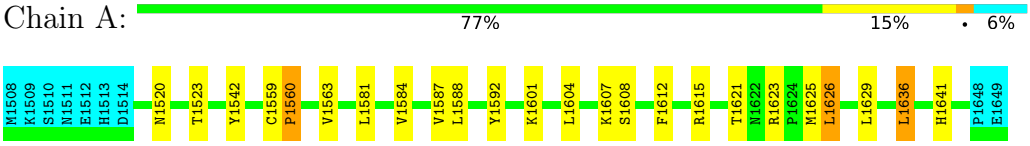
Chain B:



4.2.11 Score per residue for model 11

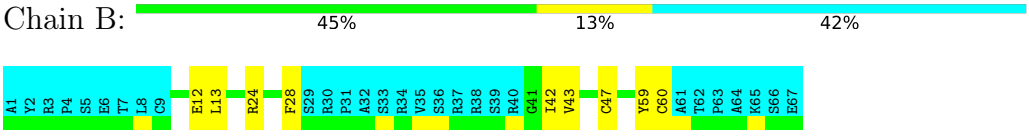
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

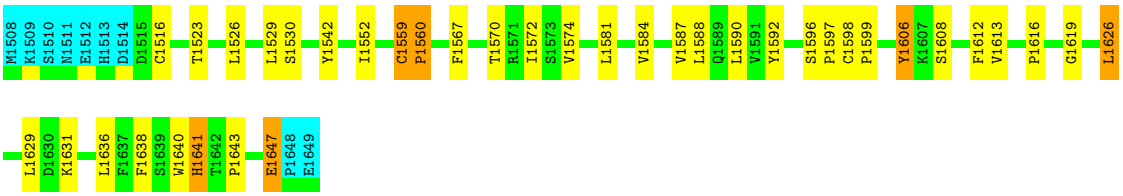
Chain B:



4.2.12 Score per residue for model 12

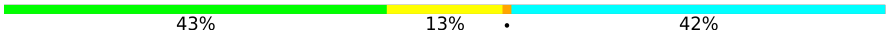
• Molecule 1: Insulin-like growth factor 2 receptor variant

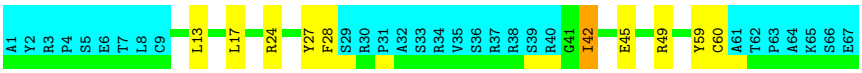
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:





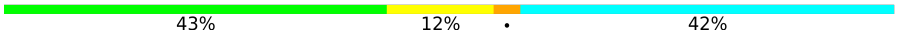
4.2.13 Score per residue for model 13

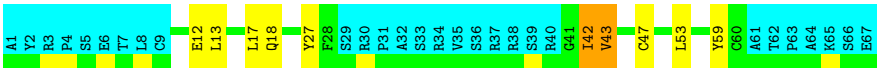
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:

• Molecule 2: Insulin-like growth factor II

Chain B:

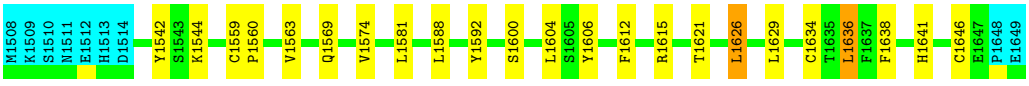




4.2.14 Score per residue for model 14

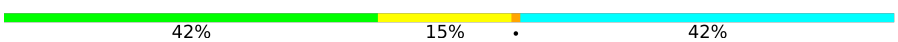
• Molecule 1: Insulin-like growth factor 2 receptor variant

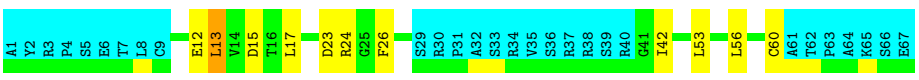
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:

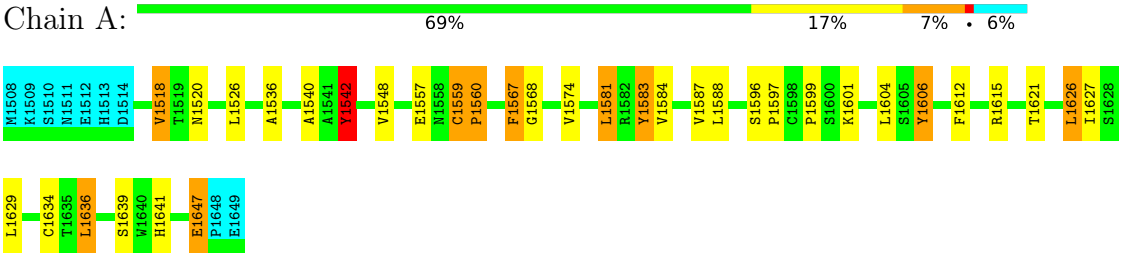




4.2.15 Score per residue for model 15

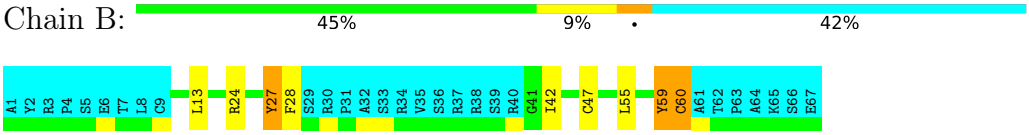
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

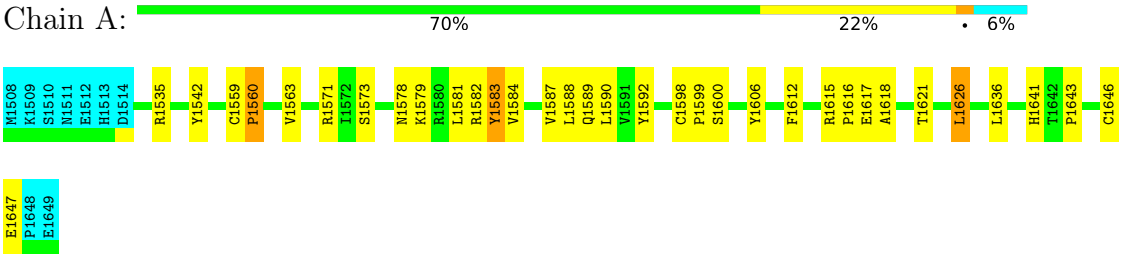
Chain B:



4.2.16 Score per residue for model 16

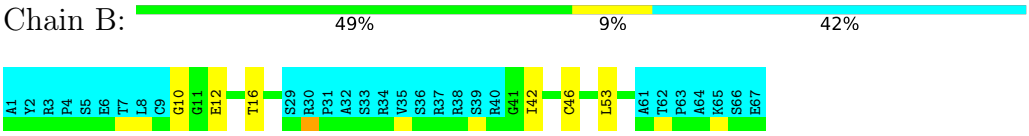
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

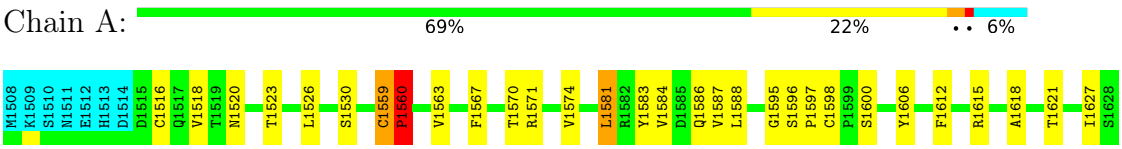
Chain B:



4.2.17 Score per residue for model 17

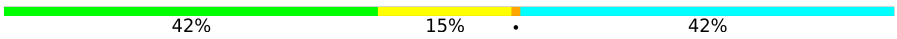
• Molecule 1: Insulin-like growth factor 2 receptor variant

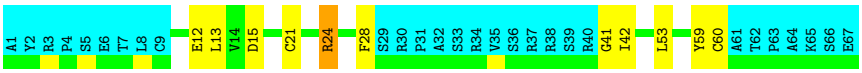
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:





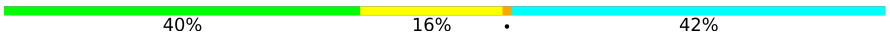
4.2.18 Score per residue for model 18

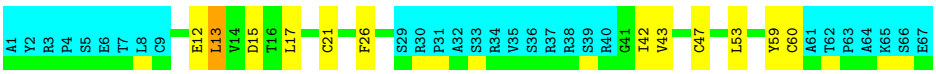
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:

• Molecule 2: Insulin-like growth factor II

Chain B:

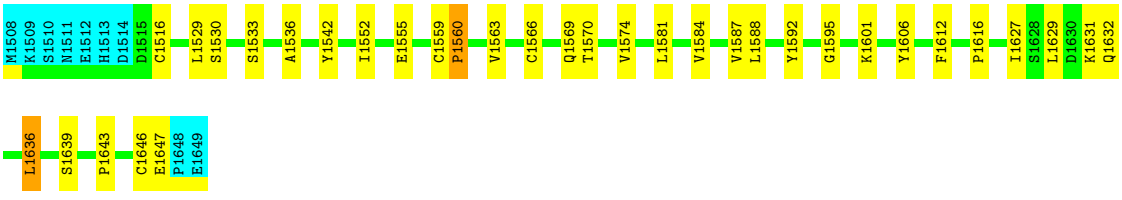




4.2.19 Score per residue for model 19

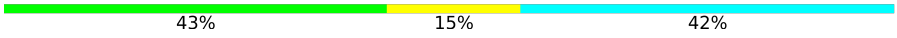
• Molecule 1: Insulin-like growth factor 2 receptor variant

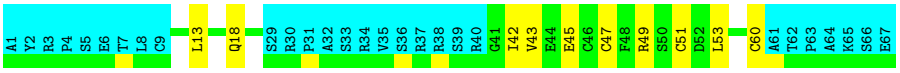
Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:

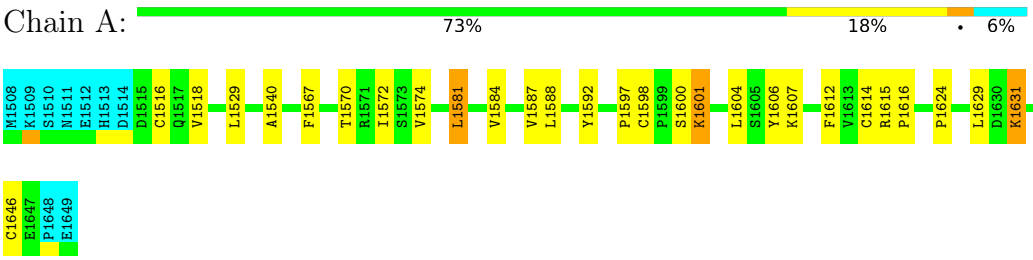




4.2.20 Score per residue for model 20

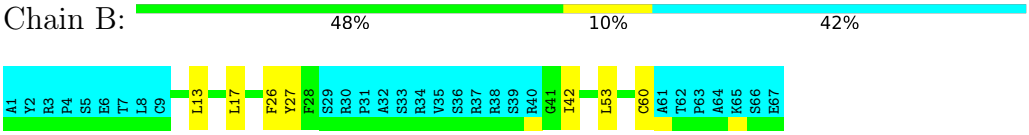
• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



• Molecule 2: Insulin-like growth factor II

Chain B:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
TALOS	geometry optimization	
iCing	refinement	r765
ARIA	refinement	2.2
ARIA	structure solution	2.2
CNS	refinement	1.2
CNS	structure solution	1.2

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2265
Number of shifts mapped to atoms	2265
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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±0.04	2±1/1026 (0.2± 0.1%)	0.97±0.03	1±1/1393 (0.1± 0.1%)
2	B	1.13±0.08	1±1/309 (0.2± 0.3%)	1.04±0.05	0±0/417 (0.0± 0.0%)
All	All	1.18	46/26700 (0.2%)	0.98	17/36200 (0.0%)

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	0.9±0.8
2	B	0.0±0.0	0.2±0.5
All	All	0	23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	27	TYR	CE1-CZ	8.48	1.58	1.38	8	2
1	A	1592	TYR	CE2-CZ	-8.41	1.18	1.38	18	4
2	B	27	TYR	CE2-CZ	-8.40	1.18	1.38	8	2
1	A	1592	TYR	CE1-CZ	7.75	1.56	1.38	18	4
1	A	1542	TYR	CE1-CZ	7.49	1.56	1.38	8	6
1	A	1542	TYR	CE2-CZ	-7.41	1.20	1.38	8	5
2	B	42	ILE	C-N	-6.43	1.27	1.33	4	1
1	A	1601	LYS	N-CA	-6.21	1.39	1.46	3	2
2	B	59	TYR	CE1-CZ	6.18	1.53	1.38	3	4
2	B	59	TYR	CE2-CZ	-6.09	1.23	1.38	3	4
1	A	1559	CYS	C-N	5.69	1.40	1.33	2	3
1	A	1583	TYR	CE2-CZ	-5.51	1.25	1.38	16	1
2	B	42	ILE	N-CA	5.45	1.53	1.46	3	1
1	A	1583	TYR	CE1-CZ	5.38	1.51	1.38	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1560	PRO	CA-C	5.30	1.57	1.52	17	2
1	A	1568	GLY	N-CA	-5.12	1.39	1.45	15	1
1	A	1567	PHE	CE1-CZ	-5.10	1.23	1.38	15	1
1	A	1545	SER	N-CA	-5.07	1.40	1.46	2	1
1	A	1567	PHE	CE2-CZ	-5.04	1.23	1.38	5	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	1638	PHE	CA-CB-CG	5.74	119.54	113.80	12	4
1	A	1559	CYS	CA-C-N	5.45	125.99	120.38	9	5
1	A	1559	CYS	C-N-CA	5.45	125.99	120.38	9	5
1	A	1619	GLY	CA-C-N	5.18	124.89	119.82	12	1
1	A	1619	GLY	C-N-CA	5.18	124.89	119.82	12	1
1	A	1592	TYR	CE1-CZ-OH	-5.14	104.47	119.90	18	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	1606	TYR	Sidechain	6
1	A	1542	TYR	Sidechain	3
1	A	1592	TYR	Sidechain	3
2	B	24	ARG	Sidechain	2
2	B	59	TYR	Sidechain	2
1	A	1615	ARG	Sidechain	1
1	A	1638	PHE	Sidechain	1
1	A	1571	ARG	Sidechain	1
1	A	1567	PHE	Sidechain	1
1	A	1527	PHE	Sidechain	1
1	A	1583	TYR	Sidechain	1
1	A	1535	ARG	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1002	983	981	16±4
2	B	303	276	276	3±2
All	All	26100	25180	25140	366

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1629:LEU:HD13	1:A:1636:LEU:HG	0.87	1.44	13	10
1:A:1588:LEU:HB2	1:A:1612:PHE:HB2	0.85	1.45	1	19
1:A:1629:LEU:HG	1:A:1636:LEU:HG	0.78	1.54	7	3
1:A:1533:SER:HA	1:A:1536:ALA:HB2	0.77	1.56	19	1
1:A:1563:VAL:HG21	1:A:1573:SER:HB2	0.76	1.58	13	2
1:A:1548:VAL:HB	1:A:1567:PHE:CE1	0.75	2.16	8	3
1:A:1600:SER:HA	2:B:53:LEU:HB2	0.73	1.59	17	5
1:A:1567:PHE:HB3	1:A:1569:GLN:HG2	0.73	1.60	4	1
1:A:1616:PRO:HA	1:A:1643:PRO:HB3	0.73	1.60	12	9
1:A:1516:CYS:HB3	1:A:1529:LEU:HB2	0.70	1.63	3	2
1:A:1621:THR:HB	1:A:1641:HIS:HB2	0.69	1.63	6	9
1:A:1627:ILE:HD11	1:A:1639:SER:HB2	0.69	1.65	1	10
1:A:1559:CYS:SG	1:A:1560:PRO:HD2	0.67	2.30	4	12
1:A:1613:VAL:HB	1:A:1641:HIS:HB3	0.67	1.65	12	1
1:A:1600:SER:HA	2:B:53:LEU:HB3	0.66	1.66	14	2
2:B:17:LEU:HD21	2:B:42:ILE:HD11	0.66	1.65	5	4
1:A:1629:LEU:HD23	1:A:1636:LEU:HG	0.65	1.68	6	1
1:A:1601:LYS:HA	1:A:1601:LYS:HE3	0.64	1.70	7	1
1:A:1632:GLN:HE21	1:A:1632:GLN:HA	0.64	1.52	10	1
1:A:1542:TYR:HE2	1:A:1626:LEU:HG	0.63	1.51	5	3
1:A:1615:ARG:HB2	1:A:1641:HIS:HB3	0.62	1.70	14	14
1:A:1629:LEU:HD13	1:A:1636:LEU:HD23	0.62	1.71	5	2
1:A:1544:LYS:HG3	2:B:23:ASP:HB3	0.61	1.71	14	1
1:A:1584:VAL:O	1:A:1587:VAL:HB	0.61	1.96	5	18
2:B:45:GLU:O	2:B:49:ARG:HG2	0.60	1.96	1	1
1:A:1542:TYR:HE1	1:A:1626:LEU:HG	0.60	1.56	15	1
2:B:53:LEU:H	2:B:53:LEU:HD12	0.59	1.58	9	1
1:A:1631:LYS:HD3	1:A:1631:LYS:H	0.59	1.58	10	3
1:A:1600:SER:HB3	2:B:53:LEU:HB2	0.59	1.74	8	2
1:A:1574:VAL:HA	1:A:1606:TYR:HB2	0.57	1.76	12	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1596:SER:HB2	1:A:1597:PRO:HD2	0.57	1.75	12	2
1:A:1559:CYS:HB3	1:A:1563:VAL:HG11	0.57	1.75	9	4
1:A:1601:LYS:HE3	2:B:53:LEU:HB3	0.56	1.77	19	1
2:B:43:VAL:O	2:B:47:CYS:HB2	0.56	2.01	19	5
1:A:1583:TYR:CE1	1:A:1586:GLN:HA	0.56	2.35	2	5
1:A:1563:VAL:HG11	1:A:1566:CYS:HB2	0.55	1.78	1	6
1:A:1600:SER:HB3	2:B:53:LEU:HD13	0.55	1.76	6	1
1:A:1516:CYS:HA	1:A:1581:LEU:HB2	0.55	1.77	8	3
1:A:1529:LEU:HG	1:A:1581:LEU:HD21	0.55	1.77	7	3
1:A:1559:CYS:HB3	1:A:1560:PRO:HD2	0.55	1.79	6	5
1:A:1573:SER:HB3	1:A:1596:SER:HB2	0.55	1.78	6	1
1:A:1582:ARG:HB2	1:A:1589:GLN:HB3	0.55	1.79	16	2
1:A:1516:CYS:SG	1:A:1529:LEU:HB2	0.55	2.42	13	1
2:B:55:LEU:O	2:B:59:TYR:HB2	0.54	2.03	15	2
1:A:1570:THR:HB	1:A:1572:ILE:HG13	0.54	1.80	20	2
1:A:1542:TYR:CE2	1:A:1626:LEU:HG	0.54	2.36	5	8
1:A:1540:ALA:HB3	1:A:1548:VAL:HG23	0.53	1.80	4	1
1:A:1590:LEU:HB3	1:A:1610:ILE:HB	0.53	1.80	1	2
1:A:1598:CYS:HA	1:A:1606:TYR:CE1	0.53	2.39	20	2
1:A:1567:PHE:HB2	1:A:1570:THR:OG1	0.53	2.04	20	2
1:A:1583:TYR:OH	1:A:1647:GLU:OE1	0.52	2.25	16	1
2:B:17:LEU:HB3	2:B:26:PHE:HB3	0.52	1.82	20	2
1:A:1600:SER:HB2	2:B:53:LEU:HG	0.52	1.81	9	1
1:A:1614:CYS:HB2	1:A:1646:CYS:HA	0.52	1.81	20	1
2:B:42:ILE:HA	2:B:45:GLU:HG2	0.51	1.83	4	1
1:A:1542:TYR:CE1	1:A:1626:LEU:HG	0.51	2.40	15	2
2:B:54:ALA:O	2:B:58:THR:HG22	0.51	2.06	1	2
1:A:1574:VAL:HA	1:A:1606:TYR:CB	0.51	2.34	19	3
1:A:1598:CYS:HA	1:A:1606:TYR:CE2	0.51	2.40	16	4
1:A:1540:ALA:HB2	1:A:1624:PRO:HG2	0.50	1.81	5	2
1:A:1569:GLN:HB3	2:B:15:ASP:OD1	0.50	2.06	18	3
2:B:26:PHE:HA	2:B:60:CYS:SG	0.50	2.47	14	2
1:A:1643:PRO:HA	1:A:1646:CYS:SG	0.50	2.46	2	3
1:A:1601:LYS:HG2	1:A:1604:LEU:HD22	0.50	1.83	20	2
1:A:1520:ASN:ND2	1:A:1583:TYR:OH	0.50	2.45	15	1
1:A:1604:LEU:HD23	1:A:1634:CYS:SG	0.50	2.47	14	3
1:A:1599:PRO:HD3	1:A:1606:TYR:OH	0.50	2.07	3	1
1:A:1523:THR:HG21	1:A:1647:GLU:HG3	0.49	1.84	3	2
1:A:1536:ALA:HB1	1:A:1552:ILE:H	0.49	1.68	19	1
1:A:1569:GLN:HB2	2:B:15:ASP:OD2	0.49	2.07	10	1
1:A:1599:PRO:HD2	1:A:1606:TYR:HE1	0.49	1.67	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1583:TYR:CZ	1:A:1586:GLN:HA	0.49	2.43	3	1
1:A:1631:LYS:HB2	2:B:53:LEU:HD21	0.49	1.83	4	1
1:A:1516:CYS:HA	1:A:1581:LEU:HD23	0.49	1.83	20	1
1:A:1530:SER:HA	1:A:1533:SER:OG	0.49	2.07	18	3
1:A:1552:ILE:HG13	1:A:1640:TRP:HZ3	0.49	1.67	12	1
1:A:1596:SER:HB3	1:A:1597:PRO:HD2	0.49	1.85	17	1
1:A:1560:PRO:O	1:A:1563:VAL:HG12	0.49	2.08	14	1
1:A:1533:SER:HA	1:A:1552:ILE:HB	0.49	1.84	1	1
2:B:17:LEU:O	2:B:21:CYS:HB2	0.49	2.06	8	4
1:A:1631:LYS:HB2	2:B:53:LEU:CD2	0.48	2.37	4	1
1:A:1518:VAL:HG21	1:A:1583:TYR:HB2	0.48	1.85	15	4
1:A:1601:LYS:HA	1:A:1601:LYS:HE2	0.48	1.85	20	1
1:A:1598:CYS:HA	1:A:1606:TYR:HE1	0.48	1.67	12	1
1:A:1600:SER:HB3	2:B:53:LEU:HB3	0.48	1.83	16	1
1:A:1546:GLY:HA3	1:A:1569:GLN:HG2	0.48	1.86	10	1
1:A:1599:PRO:HB2	2:B:16:THR:HB	0.48	1.84	16	1
1:A:1629:LEU:HG	1:A:1636:LEU:CD2	0.48	2.38	12	1
2:B:42:ILE:HA	2:B:45:GLU:CG	0.47	2.38	4	1
1:A:1563:VAL:HG21	1:A:1573:SER:CB	0.47	2.37	13	1
1:A:1625:MET:HB2	1:A:1639:SER:HB3	0.47	1.86	1	1
1:A:1631:LYS:HB3	2:B:53:LEU:HD22	0.47	1.87	9	1
2:B:11:GLY:O	2:B:15:ASP:HB2	0.47	2.10	4	1
1:A:1560:PRO:O	1:A:1563:VAL:HB	0.47	2.10	11	1
1:A:1593:LYS:HB3	1:A:1607:LYS:HD3	0.47	1.85	6	1
1:A:1545:SER:HB2	1:A:1569:GLN:HG2	0.47	1.85	13	1
1:A:1600:SER:HB2	1:A:1634:CYS:SG	0.47	2.50	18	1
1:A:1516:CYS:O	1:A:1529:LEU:HB2	0.46	2.11	12	1
1:A:1632:GLN:HE21	1:A:1632:GLN:CA	0.46	2.23	10	1
1:A:1592:TYR:O	1:A:1607:LYS:HG3	0.46	2.10	1	1
1:A:1615:ARG:CB	1:A:1641:HIS:HB3	0.46	2.41	16	1
2:B:28:PHE:O	2:B:41:GLY:HA3	0.46	2.10	17	1
1:A:1612:PHE:HE1	1:A:1640:TRP:CE3	0.46	2.28	12	1
2:B:13:LEU:O	2:B:17:LEU:HD23	0.46	2.10	18	2
1:A:1563:VAL:CG1	1:A:1566:CYS:HB2	0.46	2.40	1	3
1:A:1614:CYS:SG	1:A:1616:PRO:HD3	0.46	2.50	20	2
1:A:1529:LEU:HG	1:A:1581:LEU:HD11	0.46	1.87	1	1
1:A:1599:PRO:HD2	1:A:1606:TYR:CE1	0.45	2.46	12	1
2:B:28:PHE:HA	2:B:59:TYR:HE2	0.45	1.71	12	1
1:A:1525:HIS:CE1	1:A:1647:GLU:HB3	0.45	2.46	4	1
2:B:17:LEU:HB3	2:B:26:PHE:CB	0.45	2.42	7	1
1:A:1592:TYR:HB2	1:A:1608:SER:HB3	0.45	1.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1599:PRO:HD2	1:A:1606:TYR:OH	0.45	2.12	15	1
1:A:1597:PRO:HA	1:A:1604:LEU:O	0.45	2.12	1	2
1:A:1560:PRO:HD2	1:A:1571:ARG:HB3	0.45	1.89	8	1
1:A:1623:ARG:O	1:A:1625:MET:HG3	0.44	2.12	11	2
1:A:1583:TYR:HE1	1:A:1586:GLN:HA	0.44	1.71	7	1
2:B:24:ARG:HG2	2:B:60:CYS:SG	0.44	2.52	8	1
2:B:45:GLU:O	2:B:49:ARG:HB2	0.44	2.12	12	3
1:A:1533:SER:HA	1:A:1552:ILE:O	0.44	2.12	7	1
1:A:1598:CYS:SG	1:A:1600:SER:HB2	0.44	2.53	17	1
1:A:1515:ASP:O	1:A:1579:LYS:HB3	0.44	2.13	6	1
1:A:1570:THR:HA	2:B:15:ASP:OD2	0.44	2.12	17	1
1:A:1582:ARG:HD2	1:A:1589:GLN:OE1	0.43	2.13	4	1
1:A:1618:ALA:HB2	1:A:1643:PRO:HG3	0.43	1.89	17	1
1:A:1629:LEU:HD13	1:A:1636:LEU:CD2	0.43	2.43	4	2
1:A:1583:TYR:OH	1:A:1647:GLU:OE2	0.43	2.32	15	1
1:A:1629:LEU:CG	1:A:1636:LEU:HG	0.43	2.36	7	1
1:A:1615:ARG:HG3	1:A:1617:GLU:HB3	0.43	1.89	16	1
1:A:1518:VAL:CG2	1:A:1581:LEU:HD12	0.43	2.44	7	2
2:B:24:ARG:HD2	2:B:60:CYS:SG	0.43	2.54	15	1
1:A:1569:GLN:NE2	2:B:18:GLN:HE22	0.43	2.12	19	1
2:B:53:LEU:HD23	2:B:53:LEU:H	0.42	1.74	3	1
1:A:1536:ALA:HA	1:A:1557:GLU:HG2	0.42	1.92	15	1
1:A:1600:SER:HB3	2:B:53:LEU:CB	0.42	2.44	16	1
1:A:1606:TYR:HD1	1:A:1636:LEU:HD11	0.42	1.74	17	1
1:A:1542:TYR:HE2	1:A:1626:LEU:HD13	0.42	1.73	18	1
2:B:28:PHE:HD2	2:B:41:GLY:H	0.42	1.57	7	1
1:A:1631:LYS:N	1:A:1631:LYS:HD3	0.42	2.30	20	1
1:A:1520:ASN:OD1	1:A:1523:THR:HG22	0.42	2.14	11	4
1:A:1629:LEU:CD1	1:A:1636:LEU:HG	0.42	2.44	8	1
1:A:1592:TYR:HB2	1:A:1608:SER:HB2	0.42	1.92	11	1
1:A:1545:SER:HB3	2:B:18:GLN:CD	0.42	2.40	13	1
1:A:1578:ASN:O	1:A:1592:TYR:HE1	0.42	1.98	16	1
2:B:21:CYS:HA	2:B:24:ARG:HB3	0.41	1.92	17	1
2:B:28:PHE:HA	2:B:59:TYR:CE2	0.41	2.50	12	1
1:A:1549:TYR:HB3	1:A:1556:ASN:ND2	0.41	2.30	7	1
1:A:1624:PRO:HA	1:A:1639:SER:O	0.41	2.15	7	1
1:A:1542:TYR:HD2	1:A:1567:PHE:CZ	0.41	2.34	4	1
1:A:1581:LEU:HA	1:A:1589:GLN:O	0.41	2.16	2	1
1:A:1567:PHE:CE2	1:A:1574:VAL:HG11	0.41	2.51	12	1
1:A:1540:ALA:HB3	1:A:1548:VAL:CG1	0.41	2.45	15	1
1:A:1540:ALA:HB3	1:A:1548:VAL:HG12	0.41	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1580:ARG:NE	1:A:1580:ARG:HA	0.41	2.31	2	1
2:B:21:CYS:HB2	2:B:26:PHE:HB3	0.41	1.92	18	1
1:A:1601:LYS:HB3	1:A:1604:LEU:HD22	0.41	1.93	11	1
1:A:1573:SER:O	1:A:1596:SER:HB3	0.40	2.16	6	1
1:A:1601:LYS:HE3	1:A:1604:LEU:HD13	0.40	1.92	15	1
1:A:1536:ALA:HB1	1:A:1552:ILE:N	0.40	2.31	19	1
1:A:1573:SER:HB3	1:A:1596:SER:OG	0.40	2.16	9	1
1:A:1563:VAL:CG2	1:A:1573:SER:HB2	0.40	2.40	13	2
1:A:1592:TYR:O	1:A:1607:LYS:HA	0.40	2.16	20	1
1:A:1615:ARG:HD2	1:A:1617:GLU:OE1	0.40	2.16	13	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	133/142 (94%)	119±3 (89±2%)	13±3 (10±2%)	1±1 (1±1%)	14	63
2	B	39/67 (58%)	34±2 (87±5%)	3±2 (9±4%)	2±1 (4±2%)	3	27
All	All	3440/4180 (82%)	3048 (89%)	329 (10%)	63 (2%)	9	52

All 10 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	1560	PRO	17
2	B	42	ILE	16
2	B	60	CYS	14
1	A	1618	ALA	4
2	B	28	PHE	3
1	A	1595	GLY	3
2	B	10	GLY	2
1	A	1542	TYR	2
1	A	1515	ASP	1
1	A	1577	ALA	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	114/123 (93%)	108±1 (95±1%)	6±1 (5±1%)	24 75
2	B	33/57 (58%)	32±1 (97±2%)	1±1 (3±2%)	35 84
All	All	2940/3600 (82%)	2809 (96%)	131 (4%)	26 77

All 36 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	1581	LEU	19
1	A	1636	LEU	17
2	B	13	LEU	12
1	A	1626	LEU	11
1	A	1647	GLU	8
1	A	1601	LYS	5
1	A	1526	LEU	5
1	A	1530	SER	5
1	A	1607	LYS	4
1	A	1571	ARG	4
1	A	1570	THR	3
1	A	1631	LYS	3
1	A	1590	LEU	3
1	A	1569	GLN	2
1	A	1580	ARG	2
2	B	43	VAL	2
1	A	1555	GLU	2
1	A	1574	VAL	2
2	B	56	LEU	2
1	A	1563	VAL	2
1	A	1632	GLN	2
1	A	1518	VAL	2
1	A	1539	THR	1
1	A	1544	LYS	1
1	A	1604	LEU	1
1	A	1576	LYS	1
1	A	1548	VAL	1
2	B	45	GLU	1

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Mol	Chain	Res	Type	Models (Total)
2	B	28	PHE	1
1	A	1615	ARG	1
2	B	17	LEU	1
1	A	1557	GLU	1
1	A	1641	HIS	1
2	B	24	ARG	1
2	B	59	TYR	1
1	A	1614	CYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% 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	2265
Number of shifts mapped to atoms	2265
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	198	-0.06 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	172	0.26 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	178	0.21 ± 0.11	None needed (< 0.5 ppm)
^{15}N	188	0.48 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1862 atoms were assigned a chemical shift out of a possible 2214. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	801/859 (93%)	336/352 (95%)	306/344 (89%)	159/163 (98%)
Sidechain	928/1164 (80%)	637/760 (84%)	272/362 (75%)	19/42 (45%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	133/191 (70%)	82/92 (89%)	50/94 (53%)	1/5 (20%)
Overall	1862/2214 (84%)	1055/1204 (88%)	628/800 (78%)	179/210 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 2263 atoms were assigned a chemical shift out of a possible 2708. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	965/1036 (93%)	401/422 (95%)	376/418 (90%)	188/196 (96%)
Sidechain	1161/1464 (79%)	793/951 (83%)	342/450 (76%)	26/63 (41%)
Aromatic	137/208 (66%)	86/100 (86%)	50/101 (50%)	1/7 (14%)
Overall	2263/2708 (84%)	1280/1473 (87%)	768/969 (79%)	215/266 (81%)

7.1.4 Statistically unusual chemical shifts (i)

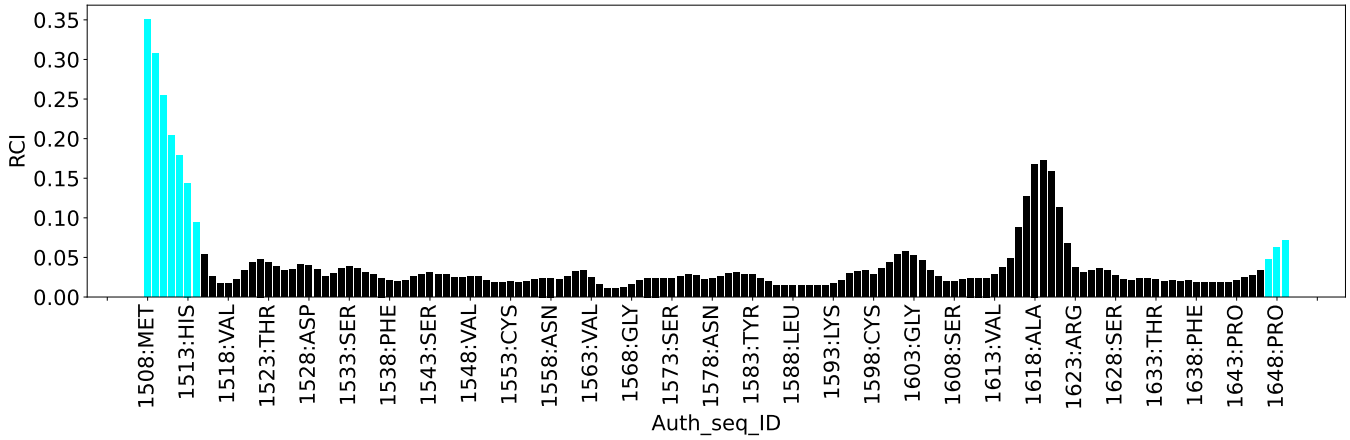
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1572	ILE	HB	0.06	0.35 – 3.22	-6.0

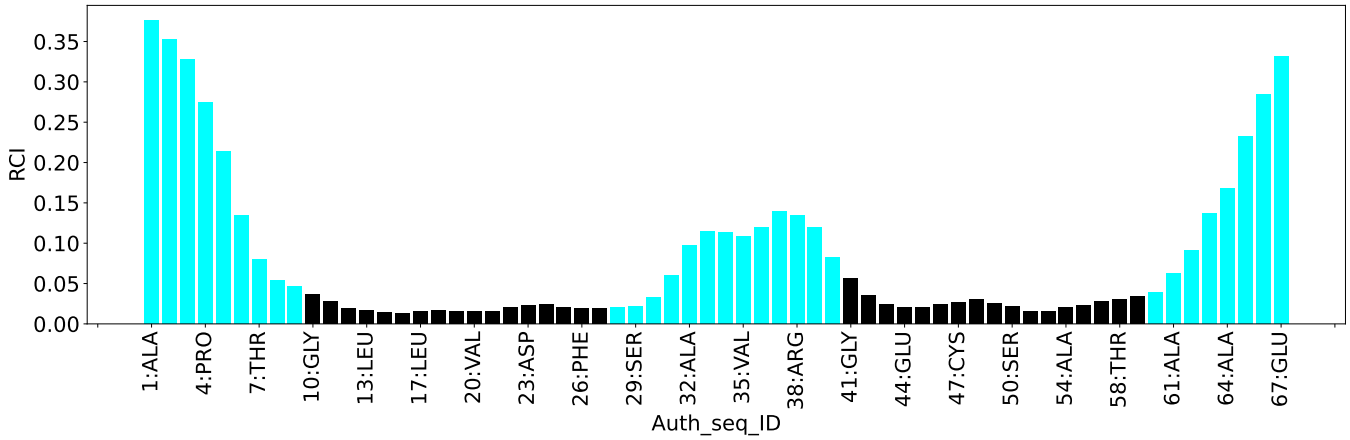
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3071
Intra-residue (|i-j|=0)	1109
Sequential (|i-j|=1)	845
Medium range (|i-j|>1 and |i-j|<5)	338
Long range (|i-j|≥5)	688
Inter-chain	42
Hydrogen bond restraints	49
Disulfide bond restraints	0
Total dihedral-angle restraints	318
Number of unmapped restraints	0
Number of restraints per residue	16.2
Number of long range restraints per residue[1]	3.5

[1]Long 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)	88.2	0.2
0.2-0.5 (Medium)	186.9	0.5
>0.5 (Large)	191.8	4.61

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.2	5.72
10.0-20.0 (Medium)	0.1	14.02
>20.0 (Large)	None	None

9 Distance violation analysis (i)

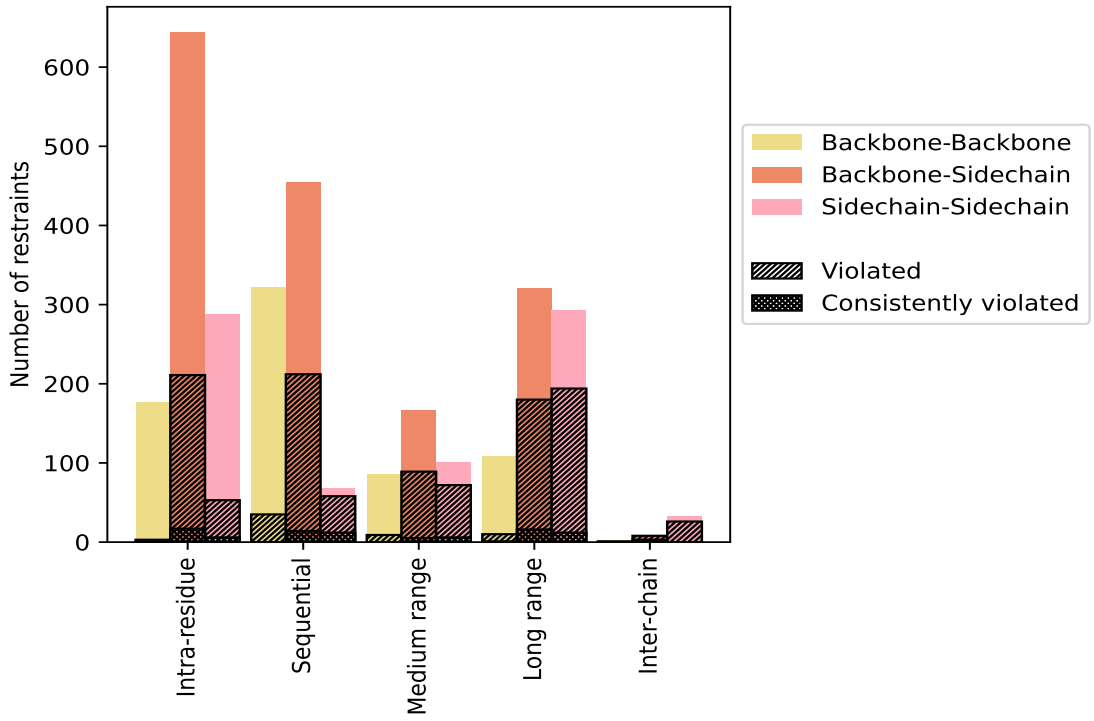
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1109	36.1	267	24.1	8.7	24	2.2	0.8
Backbone-Backbone	177	5.8	3	1.7	0.1	1	0.6	0.0
Backbone-Sidechain	644	21.0	211	32.8	6.9	17	2.6	0.6
Sidechain-Sidechain	288	9.4	53	18.4	1.7	6	2.1	0.2
Sequential (|i-j|=1)	845	27.5	305	36.1	9.9	26	3.1	0.8
Backbone-Backbone	322	10.5	35	10.9	1.1	0	0.0	0.0
Backbone-Sidechain	455	14.8	212	46.6	6.9	14	3.1	0.5
Sidechain-Sidechain	68	2.2	58	85.3	1.9	12	17.6	0.4
Medium range (|i-j|>1 & |i-j|<5)	338	11.0	168	49.7	5.5	11	3.3	0.4
Backbone-Backbone	86	2.8	9	10.5	0.3	0	0.0	0.0
Backbone-Sidechain	151	4.9	87	57.6	2.8	5	3.3	0.2
Sidechain-Sidechain	101	3.3	72	71.3	2.3	6	5.9	0.2
Long range (|i-j|≥5)	688	22.4	383	55.7	12.5	29	4.2	0.9
Backbone-Backbone	108	3.5	10	9.3	0.3	1	0.9	0.0
Backbone-Sidechain	287	9.3	179	62.4	5.8	16	5.6	0.5
Sidechain-Sidechain	293	9.5	194	66.2	6.3	12	4.1	0.4
Inter-chain	42	1.4	35	83.3	1.1	3	7.1	0.1
Backbone-Backbone	2	0.1	1	50.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.3	8	100.0	0.3	3	37.5	0.1
Sidechain-Sidechain	32	1.0	26	81.2	0.8	0	0.0	0.0
Hydrogen bond	49	1.6	3	6.1	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3071	100.0	1161	37.8	37.8	93	3.0	3.0
Backbone-Backbone	695	22.6	58	8.3	1.9	2	0.3	0.1
Backbone-Sidechain	1594	51.9	700	43.9	22.8	55	3.5	1.8
Sidechain-Sidechain	782	25.5	403	51.5	13.1	36	4.6	1.2

[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



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

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	108	126	78	153	10	475	0.53	3.09	0.43	0.42
2	105	122	68	151	12	458	0.53	4.31	0.46	0.44
3	110	128	66	134	9	447	0.5	2.98	0.35	0.42
4	111	139	72	152	8	482	0.52	3.31	0.41	0.41
5	114	122	63	151	12	462	0.6	4.56	0.54	0.44
6	106	134	74	149	11	474	0.51	2.83	0.36	0.44
7	107	125	73	174	7	486	0.54	3.27	0.47	0.41
8	104	124	72	155	10	465	0.51	3.02	0.39	0.4
9	99	124	67	167	15	472	0.51	3.18	0.38	0.41
10	107	126	74	149	13	469	0.5	2.23	0.36	0.4

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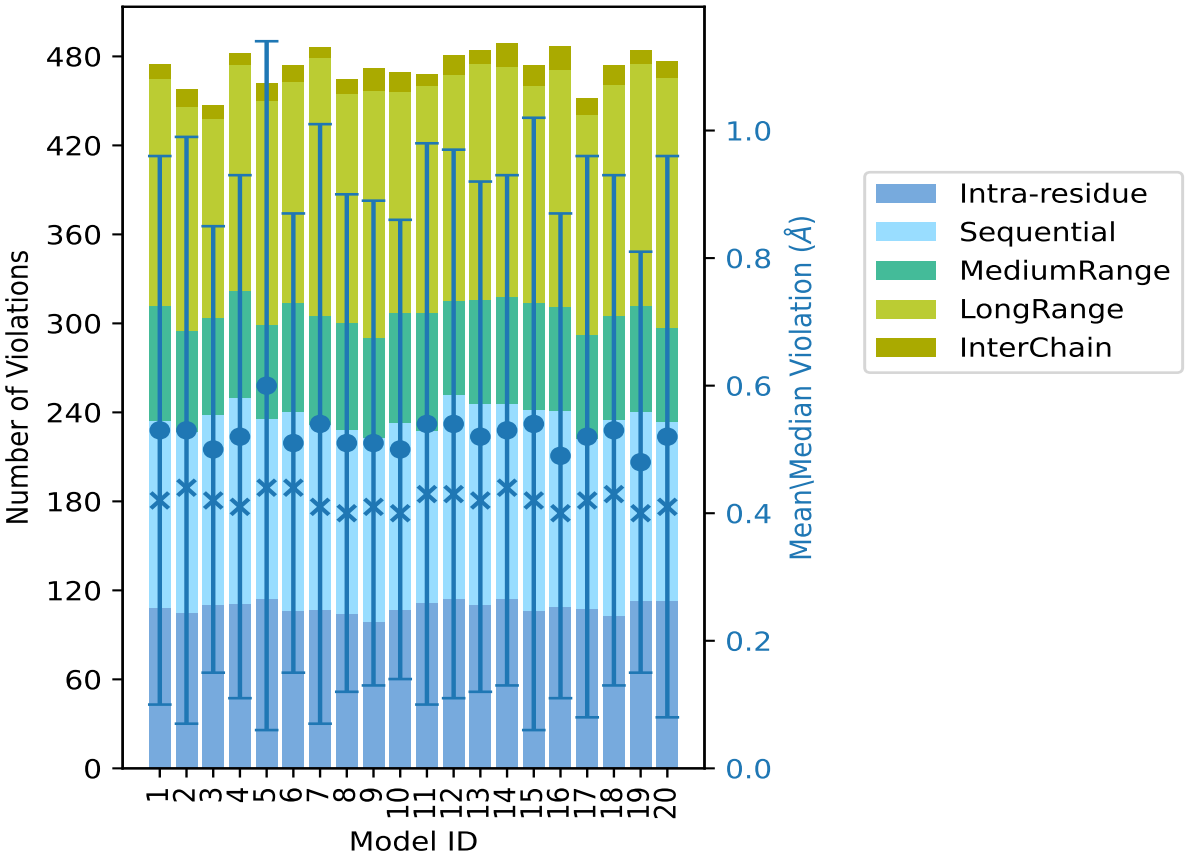
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	112	116	79	153	8	468	0.54	3.49	0.44	0.43
12	114	138	63	153	13	481	0.54	3.03	0.43	0.43
13	110	136	70	159	9	484	0.52	3.29	0.4	0.42
14	114	132	72	155	16	489	0.53	3.57	0.4	0.44
15	106	136	72	146	14	474	0.54	4.03	0.48	0.42
16	109	132	70	160	16	487	0.49	3.04	0.38	0.4
17	108	114	70	149	11	452	0.52	4.61	0.44	0.42
18	103	132	70	156	13	474	0.53	2.89	0.4	0.43
19	113	127	72	163	9	484	0.48	2.24	0.33	0.4
20	113	121	63	169	11	477	0.52	3.71	0.44	0.41

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

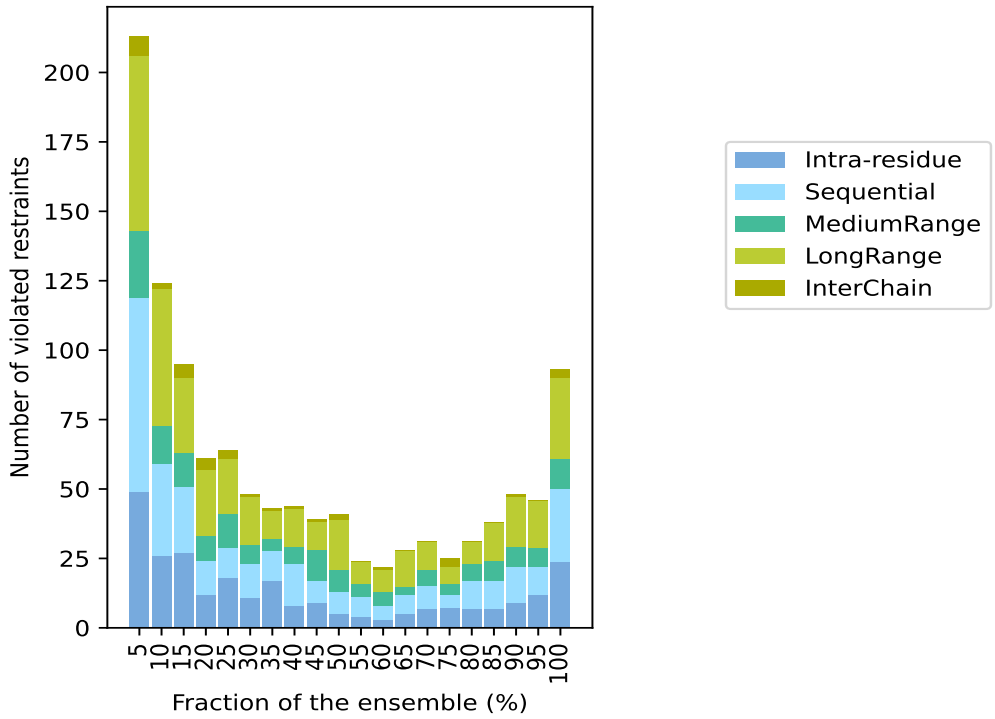
9.3 Distance violation statistics for the ensemble (i)

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, 1864(IR:842, SQ:540, MR:170, LR:305, IC:7) 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]	%
49	70	24	63	7	213	1	5.0
26	33	14	49	2	124	2	10.0
27	24	12	27	5	95	3	15.0
12	12	9	24	4	61	4	20.0
18	11	12	20	3	64	5	25.0
11	12	7	17	1	48	6	30.0
17	11	4	10	1	43	7	35.0
8	15	6	14	1	44	8	40.0
9	8	11	10	1	39	9	45.0
5	8	8	18	2	41	10	50.0
4	7	5	8	0	24	11	55.0
3	5	5	8	1	22	12	60.0
5	7	3	13	0	28	13	65.0
7	8	6	10	0	31	14	70.0
7	5	4	6	3	25	15	75.0
7	10	6	8	0	31	16	80.0
7	10	7	14	0	38	17	85.0
9	13	7	18	1	48	18	90.0
12	10	7	17	0	46	19	95.0
24	26	11	29	3	93	20	100.0

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

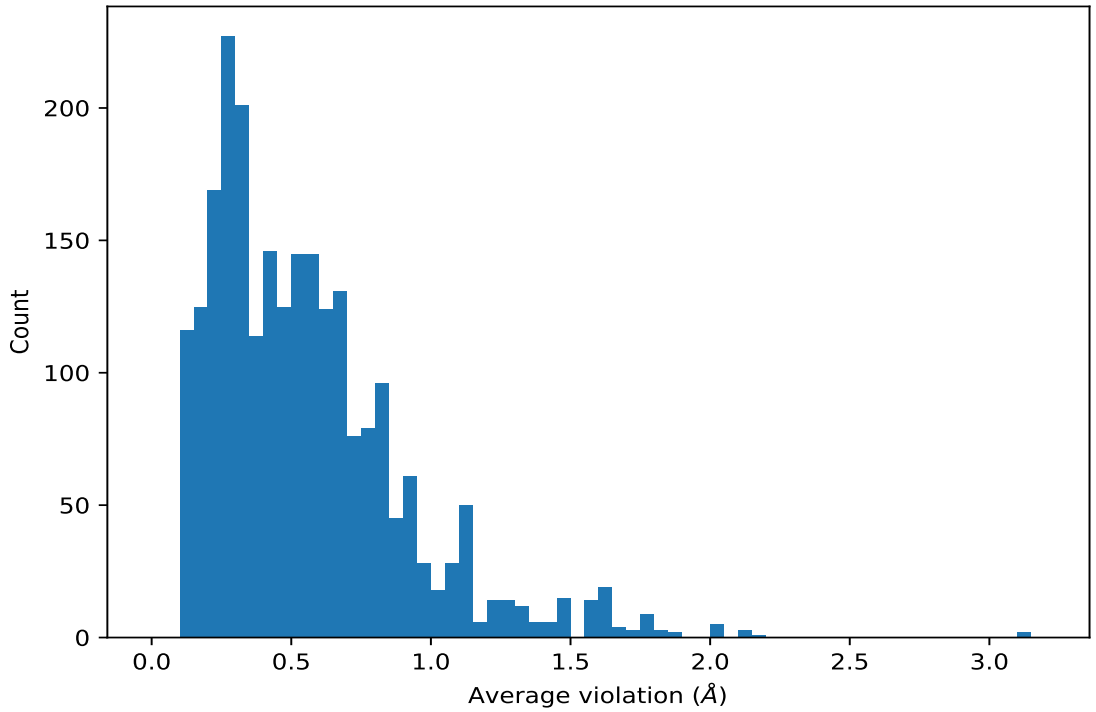
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

The following table provides the mean and the standard deviation of theviolation 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)
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	20	1.81	0.69	2.12
(1,271)	2:54:B:ALA:HB1	2:53:B:LEU:HD12	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB2	2:56:B:LEU:HD22	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD23	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB1	2:56:B:LEU:HD23	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB2	2:56:B:LEU:HD21	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD21	20	1.77	0.56	1.95
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD22	20	1.77	0.56	1.95
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	20	1.73	0.3	1.85
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	20	1.73	0.3	1.85
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	20	1.73	0.3	1.85
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	20	1.41	1.37	0.9
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD1	20	1.41	1.37	0.9
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	20	1.41	1.37	0.9

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD2	20	1.41	1.37	0.9
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD2	20	1.41	1.37	0.9
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD1	20	1.41	1.37	0.9
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	20	1.35	0.23	1.42
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	20	1.35	0.23	1.42
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	20	1.35	0.23	1.42
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD12	20	1.35	0.23	1.42
(1,505)	1:1618:A:ALA:HB3	1:1616:A:PRO:HD2	20	1.25	0.24	1.37
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	20	1.25	0.24	1.37
(1,505)	1:1618:A:ALA:HB1	1:1616:A:PRO:HD2	20	1.25	0.24	1.37
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	20	1.17	0.23	1.23
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	20	1.17	0.23	1.23
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	20	1.17	0.23	1.23
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD12	20	1.17	0.23	1.23
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD11	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD12	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD12	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD13	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD11	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD11	20	1.12	0.37	1.0
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD13	20	1.12	0.37	1.0
(1,2482)	2:13:B:LEU:HD11	2:12:B:GLU:HB3	20	1.11	0.54	1.17
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	20	1.11	0.54	1.17
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	20	1.11	0.54	1.17
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD11	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD11	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD13	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD13	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD12	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD11	1:1532:A:LEU:HD23	20	1.07	0.19	1.06
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD11	20	1.07	0.19	1.06
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	20	1.05	0.06	1.05
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	20	1.05	0.06	1.05
(1,496)	1:1627:A:ILE:HG21	1:1638:A:PHE:HA	20	1.05	0.06	1.05
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	20	1.05	0.29	1.02
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB3	20	1.05	0.29	1.02
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB2	20	1.05	0.29	1.02
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	20	1.05	0.29	1.02
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB2	20	1.05	0.29	1.02
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD12	20	1.01	0.15	1.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD13	20	1.01	0.15	1.06
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD21	20	1.01	0.15	1.06
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD11	20	1.01	0.15	1.06
(1,229)	2:55:B:LEU:HD12	2:56:B:LEU:H	20	1.01	0.15	1.06
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD23	20	1.01	0.15	1.06
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD22	20	1.01	0.15	1.06
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD1	20	0.95	0.25	1.0
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	20	0.95	0.25	1.0
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD2	20	0.95	0.25	1.0
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD1	20	0.95	0.25	1.0
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD1	20	0.95	0.25	1.0
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD2	20	0.95	0.25	1.0
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	20	0.94	0.1	0.9
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	20	0.94	0.1	0.9
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	20	0.93	0.03	0.94
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	20	0.93	0.03	0.94
(1,1961)	1:1587:A:VAL:HG12	1:1586:A:GLN:H	20	0.93	0.03	0.94
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	20	0.93	0.19	0.96
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD23	20	0.93	0.19	0.96
(2,1)	1:1574:A:VAL:HG23	1:1636:A:LEU:H	20	0.93	0.19	0.96
(2,1)	1:1574:A:VAL:HG22	1:1636:A:LEU:H	20	0.93	0.19	0.96
(2,1)	1:1574:A:VAL:HG21	1:1636:A:LEU:H	20	0.93	0.19	0.96
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD21	20	0.93	0.19	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD12	20	0.92	0.14	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD13	20	0.92	0.14	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	20	0.92	0.14	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD11	20	0.92	0.14	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD23	20	0.92	0.14	0.96
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD22	20	0.92	0.14	0.96
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	20	0.91	0.21	0.88
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	20	0.91	0.21	0.88
(1,1067)	1:1588:A:LEU:HD13	1:1583:A:TYR:HB3	20	0.91	0.21	0.88
(1,2310)	2:20:B:VAL:HG13	2:21:B:CYS:HB3	20	0.85	1.02	0.42
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	20	0.85	1.02	0.42
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	20	0.85	1.02	0.42
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	20	0.85	0.46	0.79
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	20	0.85	0.46	0.79
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	20	0.85	0.46	0.79
(1,173)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	20	0.82	0.13	0.8
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	20	0.82	0.13	0.8
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	20	0.82	0.13	0.8
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	20	0.8	0.17	0.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	20	0.8	0.17	0.76
(1,27)	1:1609:A:VAL:HG23	1:1637:A:PHE:HB3	20	0.8	0.17	0.76
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD11	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD12	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD12	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD13	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD11	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD12	20	0.8	0.16	0.81
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD13	20	0.8	0.16	0.81
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	20	0.78	0.22	0.76
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD1	20	0.78	0.22	0.76
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	20	0.78	0.22	0.76
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD2	20	0.78	0.22	0.76
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD2	20	0.78	0.22	0.76
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD2	20	0.78	0.22	0.76
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	20	0.78	0.11	0.8
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD12	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD11	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD11	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD13	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD12	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD12	20	0.76	0.51	0.7
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD13	20	0.76	0.51	0.7
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	20	0.75	0.16	0.71
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	20	0.75	0.16	0.71
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG23	20	0.75	0.16	0.71
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	20	0.75	0.15	0.8
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	20	0.75	0.15	0.8
(1,2162)	1:1548:A:VAL:HG23	1:1547:A:VAL:H	20	0.75	0.15	0.8
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	20	0.75	0.15	0.8
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	20	0.74	0.23	0.71
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG13	20	0.74	0.23	0.71
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	20	0.74	0.23	0.71
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	20	0.74	0.23	0.71
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,710)	1:1629:A:LEU:HD23	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,710)	1:1629:A:LEU:HD11	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,710)	1:1629:A:LEU:HD12	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,710)	1:1629:A:LEU:HD13	1:1629:A:LEU:H	20	0.74	0.11	0.76
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	20	0.73	0.36	0.74

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD11	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD11	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG22	1:1529:A:LEU:HD11	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG22	1:1529:A:LEU:HD12	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG22	1:1532:A:LEU:HD23	20	0.73	0.36	0.74
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD12	20	0.73	0.36	0.74
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	20	0.73	0.06	0.74
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	20	0.73	0.06	0.74
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	20	0.73	0.06	0.74
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	20	0.71	0.2	0.72
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG3	20	0.71	0.2	0.72
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	20	0.71	0.2	0.69
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	20	0.71	0.2	0.69
(1,2451)	2:62:B:THR:HG22	2:63:B:PRO:HB3	20	0.71	0.2	0.69
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	20	0.7	0.14	0.68
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	20	0.7	0.14	0.68
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	20	0.7	0.14	0.68
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD11	20	0.7	0.14	0.68
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	20	0.68	0.05	0.68
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG21	20	0.68	0.05	0.68
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	20	0.68	0.05	0.68
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	20	0.67	0.22	0.6
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE2	20	0.67	0.22	0.6
(1,39)	1:1548:A:VAL:HG23	1:1542:A:TYR:HE2	20	0.67	0.22	0.6
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE1	20	0.67	0.22	0.6
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE1	20	0.67	0.22	0.6
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	20	0.65	0.21	0.7
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	20	0.65	0.21	0.7
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	20	0.65	0.21	0.7
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	20	0.63	0.14	0.66
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG12	20	0.63	0.14	0.66
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG21	20	0.63	0.14	0.66
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	20	0.63	0.14	0.66
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	20	0.62	0.19	0.62
(1,1585)	1:1550:A:MET:H	1:1539:A:THR:HG23	20	0.62	0.19	0.62
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	20	0.62	0.19	0.62
(1,1585)	1:1550:A:MET:H	1:1539:A:THR:HG21	20	0.62	0.19	0.62
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG12	20	0.62	0.19	0.62
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	20	0.62	0.07	0.59
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	20	0.62	0.07	0.59
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	20	0.62	0.07	0.59

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	20	0.61	0.02	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	20	0.61	0.02	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	20	0.61	0.02	0.62
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	20	0.59	0.1	0.6
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	20	0.59	0.1	0.6
(1,1201)	1:1587:A:VAL:HG21	1:1584:A:VAL:H	20	0.59	0.1	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	20	0.59	0.02	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	20	0.59	0.02	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	20	0.59	0.02	0.6
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	20	0.59	0.05	0.6
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	20	0.59	0.05	0.6
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	20	0.59	0.05	0.6
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	20	0.58	0.03	0.58
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD11	20	0.58	0.55	0.38
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	20	0.58	0.55	0.38
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	20	0.58	0.55	0.38
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	20	0.57	0.2	0.6
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	20	0.57	0.2	0.6
(1,62)	1:1588:A:LEU:HD12	1:1645:A:ALA:HA	20	0.57	0.2	0.6
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	20	0.57	0.17	0.63
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	20	0.57	0.17	0.63
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	20	0.57	0.17	0.63
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	20	0.57	0.14	0.59
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	20	0.57	0.14	0.59
(1,30)	1:1587:A:VAL:HG21	1:1585:A:ASP:H	20	0.57	0.14	0.59
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	20	0.56	0.09	0.6
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	20	0.56	0.09	0.6
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	20	0.56	0.09	0.6
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	20	0.55	0.37	0.43
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	20	0.55	0.37	0.43
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	20	0.55	0.37	0.43
(1,239)	2:18:B:GLN:H	2:20:B:VAL:HG11	20	0.55	0.37	0.43
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	20	0.55	0.06	0.55
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	20	0.55	0.06	0.55
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	20	0.55	0.06	0.55
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	20	0.55	0.05	0.56
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	20	0.55	0.05	0.56
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	20	0.55	0.05	0.56
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	20	0.55	0.15	0.56
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	20	0.54	0.23	0.57
(1,199)	1:1555:A:GLU:H	1:1564:A:GLY:HA3	20	0.54	0.23	0.57
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	20	0.53	0.61	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	20	0.53	0.61	0.36
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG22	20	0.53	0.61	0.36
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	20	0.53	0.04	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	20	0.53	0.04	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	20	0.53	0.04	0.53
(1,204)	1:1610:A:ILE:HG22	1:1639:A:SER:H	20	0.5	0.16	0.51
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	20	0.5	0.16	0.51
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	20	0.5	0.16	0.51
(1,204)	1:1626:A:LEU:HD11	1:1639:A:SER:H	20	0.5	0.16	0.51
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	20	0.49	0.26	0.46
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	20	0.49	0.26	0.46
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	20	0.49	0.26	0.46
(1,1110)	1:1583:A:TYR:HD2	1:1584:A:VAL:HG22	20	0.49	0.26	0.46
(1,1110)	1:1583:A:TYR:HD2	1:1584:A:VAL:HG21	20	0.49	0.26	0.46
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	20	0.49	0.03	0.5
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	20	0.49	0.03	0.5
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	20	0.49	0.03	0.5
(1,1760)	1:1532:A:LEU:HD21	1:1533:A:SER:H	20	0.47	0.17	0.44
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	20	0.47	0.17	0.44
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	20	0.47	0.17	0.44
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	20	0.46	0.07	0.49
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	20	0.46	0.07	0.49
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	20	0.46	0.07	0.49
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	20	0.46	0.14	0.44
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG2	20	0.46	0.14	0.44
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	20	0.44	0.12	0.43
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	20	0.44	0.08	0.44
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	20	0.43	0.08	0.44
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	20	0.43	0.08	0.44
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	20	0.43	0.08	0.44
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	20	0.42	0.07	0.42
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	20	0.42	0.07	0.42
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG21	20	0.42	0.07	0.42
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	20	0.42	0.04	0.42
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD2	20	0.42	0.04	0.42
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	20	0.41	0.13	0.38
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	20	0.41	0.13	0.38
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	20	0.41	0.13	0.38
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	20	0.41	0.06	0.42
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	20	0.41	0.06	0.42
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	20	0.41	0.06	0.42
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	20	0.4	0.03	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	20	0.4	0.03	0.4
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	20	0.4	0.03	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	20	0.4	0.02	0.4
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	20	0.39	0.13	0.36
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	20	0.39	0.13	0.36
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	20	0.39	0.13	0.36
(1,490)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	20	0.39	0.13	0.36
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	20	0.39	0.13	0.36
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	20	0.39	0.13	0.36
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	20	0.39	0.14	0.38
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	20	0.39	0.14	0.38
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	20	0.39	0.14	0.38
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	20	0.38	0.03	0.37
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	20	0.38	0.03	0.37
(1,962)	1:1526:A:LEU:HD21	1:1526:A:LEU:HB3	20	0.38	0.03	0.37
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	20	0.35	0.07	0.37
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	20	0.34	0.05	0.34
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	20	0.34	0.05	0.34
(1,1045)	1:1587:A:VAL:HG12	1:1587:A:VAL:H	20	0.34	0.05	0.34
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	20	0.34	0.09	0.31
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	20	0.34	0.09	0.31
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	20	0.34	0.09	0.31
(1,183)	1:1608:A:SER:H	1:1591:A:VAL:HG12	20	0.34	0.09	0.31
(1,183)	1:1608:A:SER:H	1:1591:A:VAL:HG11	20	0.34	0.09	0.31
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	20	0.33	0.04	0.32
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	20	0.33	0.04	0.32
(1,659)	1:1526:A:LEU:HD22	1:1527:A:PHE:HA	20	0.33	0.04	0.32
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	20	0.3	0.04	0.32
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	20	0.3	0.04	0.32
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	20	0.3	0.04	0.32
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	20	0.3	0.05	0.3
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	20	0.3	0.05	0.3
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	20	0.28	0.05	0.3
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	20	0.28	0.05	0.3
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	20	0.28	0.05	0.3
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	20	0.27	0.05	0.26
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	20	0.27	0.05	0.26
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	20	0.27	0.05	0.26
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	20	0.23	0.08	0.21
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	20	0.23	0.08	0.21
(1,731)	1:1626:A:LEU:HD13	1:1626:A:LEU:H	20	0.23	0.08	0.21
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	20	0.23	0.04	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	20	0.23	0.04	0.22
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	20	0.23	0.04	0.22
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	20	0.21	0.04	0.22
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG23	20	0.21	0.04	0.22
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	20	0.21	0.04	0.22
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	20	0.21	0.04	0.22
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	20	0.21	0.03	0.22
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG21	20	0.2	0.04	0.2
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	20	0.2	0.04	0.2
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	20	0.2	0.04	0.2
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	20	0.14	0.0	0.14
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	20	0.14	0.02	0.14
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	20	0.14	0.02	0.14
(1,478)	1:1552:A:ILE:HG22	1:1552:A:ILE:HG12	20	0.14	0.02	0.14
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	19	1.49	0.85	2.06
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	19	1.49	0.85	2.06
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	19	1.49	0.85	2.06
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	19	1.13	0.26	1.2
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	19	1.13	0.26	1.2
(1,87)	1:1584:A:VAL:HG13	1:1585:A:ASP:HB2	19	1.13	0.26	1.2
(1,87)	1:1587:A:VAL:HG13	1:1612:A:PHE:HB3	19	1.13	0.26	1.2
(1,87)	1:1587:A:VAL:HG11	1:1612:A:PHE:HB3	19	1.13	0.26	1.2
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD21	19	1.12	0.47	1.11
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	19	1.12	0.47	1.11
(1,218)	1:1567:A:PHE:H	1:1548:A:VAL:HG13	19	1.12	0.47	1.11
(1,218)	1:1567:A:PHE:H	1:1548:A:VAL:HG11	19	1.12	0.47	1.11
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG21	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG23	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG21	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG23	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG22	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG23	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG21	19	0.98	0.67	0.75
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG22	19	0.98	0.67	0.75
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	19	0.89	0.2	0.91
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	19	0.89	0.2	0.91
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	19	0.89	0.2	0.91
(1,70)	1:1550:A:MET:HG3	1:1548:A:VAL:HG23	19	0.89	0.2	0.91
(1,70)	1:1550:A:MET:HG3	1:1548:A:VAL:HG21	19	0.89	0.2	0.91
(1,2232)	1:1567:A:PHE:HD2	1:1606:A:TYR:HE2	19	0.89	0.43	0.76
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	19	0.89	0.43	0.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2232)	1:1567:A:PHE:HD2	1:1542:A:TYR:HE2	19	0.89	0.43	0.76
(1,2232)	1:1567:A:PHE:HD1	1:1606:A:TYR:HE1	19	0.89	0.43	0.76
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE1	19	0.89	0.43	0.76
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG13	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG11	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG12	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD12	2:42:B:ILE:HG13	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD11	2:20:B:VAL:HG11	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD13	2:42:B:ILE:HG13	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD13	2:20:B:VAL:HG12	19	0.88	0.34	0.92
(1,2292)	2:17:B:LEU:HD13	2:20:B:VAL:HG11	19	0.88	0.34	0.92
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD2	19	0.88	0.23	0.95
(1,586)	1:1548:A:VAL:HG22	1:1638:A:PHE:HD1	19	0.88	0.23	0.95
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	19	0.88	0.23	0.95
(1,586)	1:1548:A:VAL:HG23	1:1638:A:PHE:HD2	19	0.88	0.23	0.95
(1,586)	1:1548:A:VAL:HG23	1:1638:A:PHE:HD1	19	0.88	0.23	0.95
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	19	0.85	0.12	0.86
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD2	19	0.79	0.1	0.78
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	19	0.79	0.1	0.78
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	19	0.79	0.1	0.78
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD2	19	0.79	0.1	0.78
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD1	19	0.79	0.1	0.78
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD2	19	0.79	0.1	0.78
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	19	0.75	0.48	0.65
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	19	0.75	0.48	0.65
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	19	0.75	0.48	0.65
(1,270)	2:59:B:TYR:H	2:56:B:LEU:HD22	19	0.75	0.48	0.65
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	19	0.72	0.29	0.69
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	19	0.72	0.29	0.69
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	19	0.72	0.29	0.69
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD12	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD11	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD12	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD13	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD21	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD12	1:1590:A:LEU:HD11	19	0.72	0.34	0.68
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD11	19	0.72	0.34	0.68
(1,584)	1:1540:A:ALA:HB3	1:1638:A:PHE:HD2	19	0.71	0.17	0.73
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	19	0.71	0.17	0.73
(1,584)	1:1540:A:ALA:HB3	1:1638:A:PHE:HD1	19	0.71	0.17	0.73

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	19	0.71	0.17	0.73
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD2	19	0.71	0.17	0.73
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD2	19	0.71	0.17	0.73
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD23	19	0.71	0.31	0.6
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	19	0.71	0.31	0.6
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD22	19	0.71	0.31	0.6
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	19	0.68	0.29	0.6
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HG3	19	0.68	0.29	0.6
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	19	0.66	0.21	0.71
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	19	0.66	0.21	0.71
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	19	0.66	0.21	0.71
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE2	19	0.63	0.24	0.62
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE2	19	0.63	0.24	0.62
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	19	0.63	0.24	0.62
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE1	19	0.63	0.24	0.62
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE1	19	0.63	0.24	0.62
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE1	19	0.63	0.24	0.62
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	19	0.61	0.1	0.65
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	19	0.61	0.1	0.65
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	19	0.61	0.1	0.65
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	19	0.61	0.32	0.6
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	19	0.61	0.32	0.6
(1,2481)	2:13:B:LEU:HD11	2:14:B:VAL:HB	19	0.61	0.32	0.6
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD11	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD12	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD12	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD11	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD11	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD13	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD13	19	0.55	0.24	0.53
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD12	19	0.55	0.24	0.53
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	19	0.54	0.1	0.53
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	19	0.54	0.1	0.53
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	19	0.54	0.1	0.53
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	19	0.52	0.19	0.63
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	19	0.52	0.19	0.63
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	19	0.52	0.19	0.63
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	19	0.52	0.16	0.52
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA3	19	0.52	0.16	0.52
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA2	19	0.52	0.16	0.52
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA3	19	0.52	0.16	0.52
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA2	19	0.52	0.16	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA2	19	0.52	0.16	0.52
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	19	0.51	0.12	0.52
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	19	0.49	0.1	0.51
(1,1005)	1:1532:A:LEU:HD22	1:1612:A:PHE:HZ	19	0.47	0.22	0.47
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	19	0.47	0.22	0.47
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	19	0.47	0.22	0.47
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HD1	19	0.47	0.22	0.47
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HD1	19	0.47	0.22	0.47
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD11	19	0.46	0.15	0.47
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	19	0.46	0.15	0.47
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	19	0.46	0.15	0.47
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	19	0.46	0.13	0.5
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	19	0.46	0.13	0.5
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB1	19	0.46	0.13	0.5
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD12	19	0.43	0.05	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD13	19	0.43	0.05	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	19	0.43	0.05	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD11	19	0.43	0.05	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD23	19	0.43	0.05	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD22	19	0.43	0.05	0.45
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	19	0.42	0.06	0.42
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	19	0.42	0.06	0.42
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	19	0.42	0.06	0.42
(1,1031)	1:1577:A:ALA:HB3	1:1562:A:GLY:HA3	19	0.42	0.2	0.4
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	19	0.42	0.2	0.4
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	19	0.42	0.2	0.4
(1,1157)	1:1581:A:LEU:HD13	1:1581:A:LEU:H	19	0.41	0.07	0.4
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	19	0.41	0.07	0.4
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	19	0.41	0.07	0.4
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	19	0.4	0.38	0.27
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	19	0.4	0.38	0.27
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	19	0.4	0.38	0.27
(1,297)	2:37:B:ARG:H	2:33:B:SER:HB2	19	0.39	0.12	0.39
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	19	0.39	0.12	0.39
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	19	0.39	0.12	0.39
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	19	0.37	0.41	0.3
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	19	0.37	0.41	0.3
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	19	0.37	0.41	0.3
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	19	0.36	0.05	0.36
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	19	0.36	0.05	0.36
(1,623)	1:1588:A:LEU:HD23	1:1589:A:GLN:H	19	0.36	0.05	0.36
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	19	0.33	0.19	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	19	0.31	0.15	0.29
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	19	0.31	0.15	0.29
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	19	0.31	0.15	0.29
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	19	0.3	0.06	0.32
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	19	0.3	0.06	0.32
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	19	0.3	0.06	0.32
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	19	0.3	0.13	0.26
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD1	19	0.3	0.13	0.26
(1,991)	1:1618:A:ALA:HB2	1:1617:A:GLU:HA	19	0.25	0.09	0.22
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	19	0.25	0.09	0.22
(1,991)	1:1618:A:ALA:HB3	1:1617:A:GLU:HA	19	0.25	0.09	0.22
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	19	0.24	0.04	0.23
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	19	0.24	0.04	0.23
(1,457)	1:1550:A:MET:HE3	1:1550:A:MET:HA	19	0.24	0.04	0.23
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	19	0.18	0.09	0.15
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	19	0.16	0.04	0.15
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	19	0.16	0.03	0.16
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	19	0.16	0.03	0.16
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	19	0.16	0.03	0.16
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG11	1:1565:A:ALA:HB2	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG11	1:1565:A:ALA:HB3	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB2	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB3	18	1.26	0.07	1.26
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB2	18	1.26	0.07	1.26
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG11	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG11	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD13	1:1518:A:VAL:HG12	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG12	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG12	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG13	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD13	1:1518:A:VAL:HG11	18	1.12	0.14	1.16
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG13	18	1.12	0.14	1.16
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	18	1.11	0.05	1.12
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	18	1.11	0.05	1.12
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	18	1.11	0.05	1.12
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	18	1.04	0.22	1.12
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	18	1.04	0.22	1.12
(1,10)	1:1550:A:MET:HE3	1:1549:A:TYR:HA	18	1.04	0.22	1.12
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	18	0.84	0.02	0.85
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD21	18	0.82	0.34	0.72

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	18	0.82	0.34	0.72
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD21	18	0.82	0.34	0.72
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD23	18	0.82	0.34	0.72
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD23	18	0.82	0.34	0.72
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD22	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD22	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD21	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD21	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD21	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD23	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD23	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD22	18	0.81	0.73	0.58
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD23	18	0.81	0.73	0.58
(1,226)	2:17:B:LEU:HD12	2:57:B:GLU:HA	18	0.79	0.6	0.57
(1,226)	2:17:B:LEU:HD13	2:57:B:GLU:HA	18	0.79	0.6	0.57
(1,226)	2:17:B:LEU:HD11	2:18:B:GLN:HA	18	0.79	0.6	0.57
(1,226)	2:17:B:LEU:HD12	2:18:B:GLN:HA	18	0.79	0.6	0.57
(1,226)	2:17:B:LEU:HD11	2:57:B:GLU:HA	18	0.79	0.6	0.57
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	18	0.79	0.6	0.57
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	18	0.78	0.14	0.8
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	18	0.78	0.14	0.8
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	18	0.78	0.14	0.8
(1,98)	1:1636:A:LEU:HD23	1:1606:A:TYR:HB2	18	0.73	0.18	0.68
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	18	0.73	0.18	0.68
(1,98)	1:1636:A:LEU:HD22	1:1634:A:CYS:HB3	18	0.73	0.18	0.68
(1,98)	1:1636:A:LEU:HD21	1:1634:A:CYS:HB3	18	0.73	0.18	0.68
(1,98)	1:1636:A:LEU:HD21	1:1606:A:TYR:HB2	18	0.73	0.18	0.68
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	18	0.73	0.04	0.74
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	18	0.7	0.1	0.68
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	18	0.7	0.1	0.68
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	18	0.7	0.1	0.68
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	18	0.66	0.09	0.68
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	18	0.66	0.09	0.68
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	18	0.66	0.09	0.68
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	18	0.64	0.04	0.64
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	18	0.64	0.04	0.64
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	18	0.64	0.04	0.64
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	18	0.6	0.17	0.62
(1,290)	2:26:B:PHE:H	2:18:B:GLN:H	18	0.6	0.17	0.62
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	18	0.59	0.1	0.58
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	18	0.59	0.1	0.58
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	18	0.59	0.1	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	18	0.58	0.2	0.5
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	18	0.58	0.2	0.5
(1,431)	1:1552:A:ILE:HD11	1:1610:A:ILE:HG13	18	0.58	0.2	0.5
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	18	0.57	0.71	0.4
(1,2515)	2:55:B:LEU:HD21	2:46:B:CYS:HA	18	0.57	0.71	0.4
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	18	0.57	0.71	0.4
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	18	0.56	0.15	0.57
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	18	0.56	0.15	0.57
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	18	0.55	0.15	0.55
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	18	0.55	0.15	0.55
(1,1136)	1:1590:A:LEU:HD23	1:1554:A:GLY:H	18	0.55	0.15	0.55
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	18	0.53	0.32	0.47
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	18	0.53	0.32	0.47
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	18	0.53	0.32	0.47
(1,232)	2:55:B:LEU:HD13	2:49:B:ARG:HD3	18	0.53	0.32	0.47
(1,1586)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	18	0.51	0.05	0.52
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	18	0.51	0.05	0.52
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	18	0.51	0.05	0.52
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	18	0.49	0.14	0.52
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	18	0.49	0.14	0.52
(1,2987)	2:42:B:ILE:HD13	2:56:B:LEU:HG	18	0.49	0.14	0.52
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	18	0.49	0.17	0.45
(1,228)	2:55:B:LEU:HD21	2:46:B:CYS:HA	18	0.49	0.17	0.45
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	18	0.49	0.17	0.45
(1,228)	2:55:B:LEU:HD12	2:46:B:CYS:HA	18	0.49	0.17	0.45
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	18	0.44	0.22	0.45
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	18	0.44	0.22	0.45
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	18	0.44	0.26	0.38
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	18	0.44	0.26	0.38
(1,451)	1:1550:A:MET:HE1	1:1610:A:ILE:HG13	18	0.44	0.26	0.38
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	18	0.43	0.07	0.45
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG13	18	0.37	0.29	0.26
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	18	0.37	0.29	0.26
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	18	0.37	0.29	0.26
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	18	0.37	0.17	0.3
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	18	0.37	0.17	0.3
(1,1042)	1:1609:A:VAL:HG12	1:1637:A:PHE:HB3	18	0.37	0.17	0.3
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	18	0.35	0.1	0.36
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	18	0.35	0.1	0.36
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	18	0.35	0.1	0.36
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	18	0.35	0.02	0.35
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	18	0.35	0.02	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1044)	1:1518:A:VAL:HG21	1:1582:A:ARG:HA	18	0.35	0.02	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	18	0.35	0.06	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	18	0.35	0.06	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG11	18	0.35	0.06	0.35
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	18	0.35	0.05	0.36
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	18	0.35	0.05	0.36
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD12	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD13	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD11	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD13	1:1588:A:LEU:HD13	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD11	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD12	18	0.34	0.09	0.38
(1,680)	1:1529:A:LEU:HD13	1:1588:A:LEU:HD12	18	0.34	0.09	0.38
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG23	18	0.34	0.11	0.37
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	18	0.34	0.11	0.37
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	18	0.34	0.11	0.37
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	18	0.34	0.41	0.27
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	18	0.34	0.41	0.27
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	18	0.34	0.41	0.27
(1,504)	1:1618:A:ALA:HB2	1:1619:A:GLY:HA2	18	0.34	0.13	0.38
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	18	0.34	0.13	0.38
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	18	0.34	0.13	0.38
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	18	0.32	0.05	0.34
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	18	0.32	0.05	0.34
(1,1034)	1:1518:A:VAL:HG23	1:1518:A:VAL:HA	18	0.32	0.05	0.34
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	18	0.32	0.1	0.36
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	18	0.32	0.1	0.36
(1,376)	2:54:B:ALA:HB1	2:52:B:ASP:H	18	0.32	0.1	0.36
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	18	0.3	0.29	0.26
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	18	0.3	0.29	0.26
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD13	18	0.3	0.29	0.26
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	18	0.3	0.1	0.3
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB3	18	0.3	0.1	0.3
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	18	0.3	0.1	0.3
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	18	0.29	0.06	0.3
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	18	0.28	0.09	0.26
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	18	0.28	0.09	0.26
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	18	0.28	0.09	0.26
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	18	0.28	0.09	0.27
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	18	0.28	0.09	0.27
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	18	0.28	0.09	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	18	0.26	0.1	0.31
(1,1057)	1:1626:A:LEU:HD22	1:1628:A:SER:H	18	0.26	0.1	0.31
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	18	0.26	0.1	0.31
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	18	0.2	0.02	0.2
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	18	0.2	0.02	0.2
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	18	0.2	0.02	0.2
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	18	0.16	0.01	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	18	0.16	0.01	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG22	18	0.16	0.01	0.17
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	18	0.13	0.02	0.13
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD11	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD12	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD21	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD22	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD12	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD13	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD23	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD22	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD21	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD11	17	1.55	0.58	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD13	17	1.55	0.58	1.69
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	17	1.21	0.5	1.37
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD2	17	1.06	0.21	1.12
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD2	17	1.06	0.21	1.12
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	17	1.06	0.21	1.12
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD1	17	1.06	0.21	1.12
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD1	17	1.06	0.21	1.12
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD2	17	1.06	0.21	1.12
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	17	0.94	0.34	1.02
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD11	17	0.91	0.55	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD21	17	0.91	0.55	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	17	0.91	0.55	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD23	17	0.91	0.55	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD12	17	0.91	0.55	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD22	17	0.91	0.55	0.69
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	17	0.84	0.29	0.83
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	17	0.84	0.29	0.83
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	17	0.84	0.29	0.83
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	17	0.83	0.56	0.6
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	17	0.83	0.56	0.6
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	17	0.79	0.16	0.82

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD21	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD23	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	17	0.79	0.16	0.82
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	17	0.79	0.16	0.82
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	17	0.76	0.1	0.76
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	17	0.76	0.1	0.76
(1,66)	1:1636:A:LEU:HD13	1:1638:A:PHE:HZ	17	0.76	0.1	0.76
(1,236)	2:20:B:VAL:HG11	2:19:B:PHE:HA	17	0.74	0.07	0.73
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	17	0.74	0.07	0.73
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	17	0.74	0.07	0.73
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	17	0.73	0.07	0.71
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	17	0.73	0.07	0.71
(1,2284)	2:42:B:ILE:HD12	2:42:B:ILE:H	17	0.73	0.07	0.71
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	17	0.68	0.09	0.69
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	17	0.68	0.09	0.69
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	17	0.66	0.02	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG21	17	0.66	0.02	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	17	0.66	0.02	0.66
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	17	0.66	0.27	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	17	0.66	0.27	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	17	0.66	0.27	0.59
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD23	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD21	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD21	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD22	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD22	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD22	17	0.63	0.27	0.62
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD23	17	0.63	0.27	0.62
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG22	17	0.63	0.4	0.55
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	17	0.63	0.4	0.55
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	17	0.63	0.4	0.55
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG11	17	0.63	0.4	0.55
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	17	0.63	0.13	0.65
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE2	17	0.63	0.13	0.65
(1,2848)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	17	0.63	0.13	0.65
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	17	0.63	0.13	0.65
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	17	0.63	0.13	0.65
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	17	0.53	0.25	0.58
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	17	0.53	0.25	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD22	17	0.53	0.25	0.58
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD11	17	0.53	0.25	0.58
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	17	0.52	0.02	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	17	0.52	0.02	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG22	17	0.52	0.02	0.52
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD22	17	0.51	0.1	0.56
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	17	0.51	0.1	0.56
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD21	17	0.51	0.1	0.56
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG13	17	0.5	0.02	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	17	0.5	0.02	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	17	0.5	0.02	0.51
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	17	0.49	0.17	0.55
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG3	17	0.49	0.17	0.55
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG3	17	0.49	0.17	0.55
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG2	17	0.49	0.17	0.55
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG2	17	0.49	0.17	0.55
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	17	0.48	0.26	0.4
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	17	0.48	0.26	0.4
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	17	0.48	0.26	0.4
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD11	17	0.48	0.26	0.4
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	17	0.48	0.27	0.38
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	17	0.48	0.27	0.38
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	17	0.48	0.27	0.38
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	17	0.46	0.14	0.46
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	17	0.44	0.17	0.41
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	17	0.44	0.17	0.41
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG12	17	0.44	0.17	0.41
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	17	0.43	0.1	0.47
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD13	2:26:B:PHE:HB2	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD11	2:43:B:VAL:HA	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD13	2:14:B:VAL:HA	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD12	2:14:B:VAL:HA	17	0.41	0.21	0.37
(1,245)	2:42:B:ILE:HD11	2:14:B:VAL:HA	17	0.41	0.21	0.37
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	17	0.39	0.03	0.4
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG21	17	0.39	0.03	0.4
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	17	0.39	0.03	0.4
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	17	0.39	0.14	0.39
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	17	0.38	0.14	0.35
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE2	17	0.38	0.14	0.35
(1,220)	2:6:B:GLU:HB3	2:2:B:TYR:HE1	17	0.38	0.14	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,220)	2:6:B:GLU:HB3	2:2:B:TYR:HE2	17	0.38	0.14	0.35
(1,494)	1:1610:A:ILE:HG22	1:1638:A:PHE:HD2	17	0.38	0.16	0.34
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	17	0.38	0.16	0.34
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD2	17	0.38	0.16	0.34
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD1	17	0.38	0.16	0.34
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD1	17	0.38	0.16	0.34
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	17	0.35	0.14	0.33
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	17	0.35	0.14	0.33
(1,32)	1:1547:A:VAL:HG21	1:1567:A:PHE:HB3	17	0.35	0.19	0.36
(1,32)	1:1547:A:VAL:HG23	1:1567:A:PHE:HB3	17	0.35	0.19	0.36
(1,32)	1:1547:A:VAL:HG22	1:1567:A:PHE:HB3	17	0.35	0.19	0.36
(1,32)	1:1547:A:VAL:HG21	1:1549:A:TYR:HB3	17	0.35	0.19	0.36
(1,32)	1:1547:A:VAL:HG23	1:1549:A:TYR:HB3	17	0.35	0.19	0.36
(1,32)	1:1547:A:VAL:HG22	1:1549:A:TYR:HB3	17	0.35	0.19	0.36
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	17	0.23	0.02	0.24
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	17	0.21	0.07	0.19
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	17	0.21	0.07	0.19
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	17	0.21	0.07	0.19
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	17	0.13	0.02	0.13
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	17	0.13	0.02	0.12
(1,2508)	2:14:B:VAL:HG21	2:17:B:LEU:HD13	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD13	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD13	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD11	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD12	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD12	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG21	2:17:B:LEU:HD11	16	1.48	0.97	1.15
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD11	16	1.48	0.97	1.15
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	16	0.97	0.03	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG21	16	0.97	0.03	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	16	0.97	0.03	0.97
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	16	0.91	0.13	0.93
(1,806)	1:1584:A:VAL:HG21	1:1585:A:ASP:HB2	16	0.91	0.13	0.93
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	16	0.91	0.13	0.93
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	16	0.82	0.63	0.62
(1,2277)	2:42:B:ILE:HD11	2:45:B:GLU:HB2	16	0.82	0.63	0.62
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	16	0.82	0.63	0.62
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	16	0.78	0.16	0.8
(1,1022)	1:1552:A:ILE:HD13	1:1550:A:MET:HB3	16	0.78	0.16	0.8
(1,1022)	1:1552:A:ILE:HD11	1:1550:A:MET:HB3	16	0.78	0.16	0.8
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	16	0.7	0.09	0.69
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	16	0.7	0.09	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2149)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	16	0.7	0.09	0.69
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD21	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD23	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	16	0.67	0.08	0.68
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	16	0.67	0.08	0.68
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	16	0.64	0.24	0.64
(1,329)	2:59:B:TYR:HD2	2:58:B:THR:H	16	0.64	0.24	0.64
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	16	0.64	0.24	0.64
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	16	0.63	0.03	0.62
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	16	0.63	0.03	0.62
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	16	0.63	0.03	0.62
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	16	0.62	0.39	0.55
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	16	0.61	0.12	0.61
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	16	0.61	0.12	0.61
(1,2278)	2:42:B:ILE:HD13	2:55:B:LEU:HB3	16	0.61	0.12	0.61
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	16	0.58	0.26	0.55
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	16	0.57	0.64	0.35
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	16	0.57	0.64	0.35
(1,2463)	2:56:B:LEU:HD22	2:55:B:LEU:H	16	0.57	0.64	0.35
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	16	0.46	0.5	0.28
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	16	0.46	0.5	0.28
(1,566)	1:1548:A:VAL:HG21	1:1567:A:PHE:HB3	16	0.46	0.5	0.28
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	16	0.46	0.19	0.48
(1,2861)	2:20:B:VAL:HG23	2:19:B:PHE:HD2	16	0.46	0.19	0.48
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	16	0.46	0.19	0.48
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	16	0.45	0.19	0.45
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	16	0.45	0.19	0.45
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	16	0.43	0.15	0.42
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	16	0.43	0.15	0.42
(1,996)	1:1610:A:ILE:HD11	1:1550:A:MET:HG2	16	0.43	0.15	0.42
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	16	0.43	0.16	0.39
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	16	0.43	0.16	0.39
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD11	16	0.43	0.16	0.39
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	16	0.42	0.23	0.35
(1,2251)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	16	0.42	0.23	0.35
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	16	0.42	0.23	0.35
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	16	0.42	0.23	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE2	16	0.42	0.23	0.35
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD11	16	0.4	0.11	0.44
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	16	0.4	0.11	0.44
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	16	0.4	0.11	0.44
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	16	0.38	0.13	0.36
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	16	0.38	0.13	0.36
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	16	0.37	0.21	0.31
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	16	0.37	0.21	0.31
(1,353)	2:61:B:ALA:HB2	2:60:B:CYS:HB2	16	0.37	0.21	0.31
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	16	0.37	0.03	0.36
(1,1174)	1:1591:A:VAL:HG12	1:1592:A:TYR:H	16	0.37	0.03	0.36
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	16	0.37	0.03	0.36
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	16	0.24	0.02	0.24
(1,531)	1:1591:A:VAL:HG12	1:1591:A:VAL:HA	16	0.24	0.02	0.24
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	16	0.24	0.02	0.24
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	16	0.23	0.08	0.21
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	16	0.23	0.08	0.21
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	16	0.23	0.08	0.21
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	16	0.21	0.08	0.19
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	16	0.21	0.08	0.19
(1,3008)	2:56:B:LEU:HD21	2:17:B:LEU:H	16	0.21	0.08	0.19
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	16	0.21	0.05	0.22
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	16	0.21	0.05	0.22
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	16	0.2	0.06	0.21
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	16	0.2	0.06	0.21
(1,1203)	1:1588:A:LEU:HD23	1:1584:A:VAL:H	16	0.2	0.06	0.21
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	16	0.2	0.06	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	16	0.19	0.03	0.18
(1,630)	1:1588:A:LEU:HD22	1:1588:A:LEU:HA	16	0.13	0.01	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	16	0.13	0.01	0.13
(1,630)	1:1588:A:LEU:HD23	1:1588:A:LEU:HA	16	0.13	0.01	0.13
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG11	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG13	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG13	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG23	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG11	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG12	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG22	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG23	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG21	15	1.63	0.09	1.66
(1,450)	1:1550:A:MET:HE3	1:1548:A:VAL:HG22	15	1.63	0.09	1.66
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	15	0.85	0.12	0.83

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	15	0.85	0.12	0.83
(1,227)	2:17:B:LEU:HD21	2:26:B:PHE:HB2	15	0.85	0.12	0.83
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,395)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD1	15	0.84	0.18	0.87
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,406)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	15	0.84	0.18	0.87
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD1	15	0.84	0.18	0.87
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	15	0.81	0.44	0.6
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD22	15	0.81	0.44	0.6
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD12	15	0.81	0.44	0.6
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD13	15	0.81	0.44	0.6
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD21	15	0.81	0.44	0.6
(1,267)	2:35:B:VAL:HG23	2:37:B:ARG:HD3	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD3	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD3	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG23	2:34:B:ARG:HD3	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG21	2:37:B:ARG:HD3	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD2	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD2	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG23	2:34:B:ARG:HD2	15	0.77	0.44	0.68
(1,267)	2:35:B:VAL:HG22	2:37:B:ARG:HD3	15	0.77	0.44	0.68
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	15	0.67	0.29	0.77
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD1	15	0.66	0.2	0.67
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD1	15	0.66	0.2	0.67
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	15	0.66	0.2	0.67
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD2	15	0.66	0.2	0.67
(1,2884)	2:43:B:VAL:HG21	2:28:B:PHE:HD2	15	0.66	0.2	0.67
(1,2884)	2:43:B:VAL:HG21	2:28:B:PHE:HD1	15	0.66	0.2	0.67
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD13	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD11	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD12	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD12	2:55:B:LEU:HD13	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD11	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD12	2:55:B:LEU:HD11	15	0.58	0.19	0.66
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD13	15	0.58	0.19	0.66
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	15	0.55	0.07	0.55
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	15	0.53	0.31	0.43
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	15	0.53	0.31	0.43
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	15	0.53	0.31	0.43

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	15	0.46	0.17	0.51
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	15	0.46	0.17	0.51
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG21	15	0.46	0.17	0.51
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	15	0.46	0.3	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	15	0.46	0.3	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG21	15	0.46	0.3	0.33
(1,1789)	1:1577:A:ALA:HB2	1:1578:A:ASN:H	15	0.43	0.08	0.42
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	15	0.43	0.08	0.42
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	15	0.43	0.08	0.42
(1,2976)	2:17:B:LEU:HD22	2:17:B:LEU:HB3	15	0.42	0.02	0.43
(1,2976)	2:17:B:LEU:HD21	2:17:B:LEU:HB3	15	0.42	0.02	0.43
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	15	0.42	0.02	0.43
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	15	0.39	0.05	0.4
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	15	0.39	0.05	0.4
(1,269)	2:53:B:LEU:HD21	2:53:B:LEU:HA	15	0.39	0.05	0.4
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	15	0.33	0.11	0.36
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	15	0.33	0.11	0.36
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	15	0.33	0.12	0.32
(1,359)	2:58:B:THR:H	2:59:B:TYR:HD2	15	0.33	0.12	0.32
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	15	0.33	0.06	0.34
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD13	15	0.33	0.06	0.34
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD11	15	0.33	0.06	0.34
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	15	0.32	0.07	0.34
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	15	0.28	0.09	0.28
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG22	15	0.28	0.13	0.21
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG21	15	0.28	0.13	0.21
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	15	0.28	0.13	0.21
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	15	0.2	0.05	0.21
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	15	0.2	0.06	0.18
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	15	0.2	0.06	0.18
(1,1180)	1:1610:A:ILE:HD11	1:1610:A:ILE:H	15	0.2	0.06	0.18
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	15	0.12	0.01	0.12
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,715)	1:1604:A:LEU:HD11	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,715)	1:1604:A:LEU:HD21	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,715)	1:1604:A:LEU:HD22	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,715)	1:1604:A:LEU:HD13	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,715)	1:1604:A:LEU:HD23	1:1603:A:GLY:HA2	14	1.23	0.54	1.48
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG23	14	0.96	0.44	0.96
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG21	14	0.96	0.44	0.96
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG22	14	0.96	0.44	0.96
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	14	0.96	0.44	0.96

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG12	14	0.96	0.44	0.96
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG11	14	0.96	0.44	0.96
(1,563)	1:1591:A:VAL:HG12	1:1589:A:GLN:HE21	14	0.91	0.45	0.98
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	14	0.91	0.45	0.98
(1,563)	1:1591:A:VAL:HG13	1:1589:A:GLN:HE21	14	0.91	0.45	0.98
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	14	0.9	0.45	1.19
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	14	0.9	0.45	1.19
(1,726)	1:1604:A:LEU:HD13	1:1602:A:SER:HA	14	0.9	0.45	1.19
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG21	14	0.67	0.21	0.72
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	14	0.67	0.21	0.72
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	14	0.67	0.21	0.72
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG23	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG22	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG21	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG21	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG23	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG12	1:1539:A:THR:HG23	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG12	1:1539:A:THR:HG22	14	0.66	0.17	0.72
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG22	14	0.66	0.17	0.72
(1,129)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	14	0.62	0.05	0.62
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	14	0.62	0.05	0.62
(1,129)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	14	0.62	0.05	0.62
(1,524)	1:1577:A:ALA:HB1	1:1592:A:TYR:HE1	14	0.62	0.29	0.56
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE2	14	0.62	0.29	0.56
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	14	0.62	0.29	0.56
(1,524)	1:1577:A:ALA:HB2	1:1592:A:TYR:HE2	14	0.62	0.29	0.56
(1,524)	1:1577:A:ALA:HB1	1:1592:A:TYR:HE2	14	0.62	0.29	0.56
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	14	0.61	0.36	0.52
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD13	14	0.61	0.36	0.52
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD13	14	0.61	0.36	0.52
(1,697)	1:1644:A:LEU:HD12	1:1529:A:LEU:HD12	14	0.61	0.36	0.52
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD12	14	0.61	0.36	0.52
(1,697)	1:1644:A:LEU:HD12	1:1529:A:LEU:HD11	14	0.61	0.36	0.52
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,2439)	2:13:B:LEU:HD22	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,2841)	2:13:B:LEU:HD22	2:47:B:CYS:H	14	0.59	0.49	0.55
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	14	0.54	0.08	0.57
(1,725)	1:1581:A:LEU:HD21	1:1517:A:GLN:HA	14	0.54	0.08	0.57
(1,725)	1:1581:A:LEU:HD22	1:1517:A:GLN:HA	14	0.54	0.08	0.57

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	14	0.53	0.38	0.5
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	14	0.53	0.38	0.5
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD22	14	0.53	0.38	0.5
(1,231)	2:55:B:LEU:HD22	2:57:B:GLU:H	14	0.53	0.38	0.5
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	14	0.52	0.25	0.55
(1,1003)	1:1644:A:LEU:HD21	1:1532:A:LEU:H	14	0.52	0.25	0.55
(1,1003)	1:1644:A:LEU:HD22	1:1532:A:LEU:H	14	0.52	0.25	0.55
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	14	0.51	0.14	0.55
(1,528)	1:1570:A:THR:HG21	1:1571:A:ARG:H	14	0.51	0.14	0.55
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	14	0.51	0.14	0.55
(1,34)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	14	0.5	0.05	0.5
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	14	0.5	0.05	0.5
(1,34)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	14	0.5	0.05	0.5
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	14	0.47	0.25	0.34
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	14	0.47	0.25	0.34
(1,323)	2:60:B:CYS:H	2:56:B:LEU:HD22	14	0.47	0.25	0.34
(1,447)	1:1550:A:MET:HE3	1:1550:A:MET:HG2	14	0.47	0.01	0.47
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	14	0.47	0.01	0.47
(1,447)	1:1550:A:MET:HE1	1:1550:A:MET:HG2	14	0.47	0.01	0.47
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	14	0.43	0.16	0.52
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	14	0.35	0.13	0.3
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	14	0.33	0.1	0.32
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	14	0.3	0.07	0.32
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG22	14	0.3	0.07	0.32
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	14	0.3	0.07	0.32
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	14	0.29	0.1	0.26
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	14	0.29	0.1	0.26
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	14	0.28	0.1	0.28
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	14	0.28	0.1	0.28
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG21	14	0.28	0.1	0.28
(1,28)	1:1609:A:VAL:HG22	1:1607:A:LYS:HB3	14	0.28	0.15	0.25
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG12	14	0.28	0.15	0.25
(1,28)	1:1609:A:VAL:HG21	1:1607:A:LYS:HB3	14	0.28	0.15	0.25
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG13	14	0.28	0.15	0.25
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB3	14	0.28	0.15	0.25
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB2	14	0.28	0.15	0.25
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	14	0.27	0.12	0.26
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	14	0.27	0.12	0.26
(1,24)	1:1587:A:VAL:HG21	1:1586:A:GLN:HA	14	0.27	0.12	0.26
(1,24)	1:1587:A:VAL:HG23	1:1611:A:SER:HB2	14	0.27	0.12	0.26
(1,458)	1:1572:A:ILE:HD12	1:1572:A:ILE:H	14	0.25	0.08	0.26
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	14	0.25	0.08	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,458)	1:1572:A:ILE:HD11	1:1572:A:ILE:H	14	0.25	0.08	0.26
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	14	0.24	0.06	0.26
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG22	14	0.24	0.06	0.26
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	14	0.24	0.06	0.26
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	14	0.22	0.05	0.2
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	14	0.22	0.05	0.2
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	14	0.16	0.03	0.16
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	14	0.16	0.03	0.16
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	13	0.9	0.26	0.98
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	13	0.83	0.69	0.53
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD11	13	0.83	0.69	0.53
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	13	0.83	0.69	0.53
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	13	0.8	0.36	0.79
(1,56)	1:1563:A:VAL:HG21	1:1559:A:CYS:H	13	0.8	0.36	0.79
(1,56)	1:1563:A:VAL:HG21	1:1572:A:ILE:H	13	0.8	0.36	0.79
(1,56)	1:1563:A:VAL:HG22	1:1572:A:ILE:H	13	0.8	0.36	0.79
(1,56)	1:1563:A:VAL:HG23	1:1559:A:CYS:H	13	0.8	0.36	0.79
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE2	13	0.71	0.77	0.36
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE1	13	0.71	0.77	0.36
(1,2303)	2:20:B:VAL:HG21	2:19:B:PHE:HE2	13	0.71	0.77	0.36
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	13	0.71	0.77	0.36
(1,11)	1:1625:A:MET:HE3	1:1626:A:LEU:HA	13	0.7	0.42	0.55
(1,11)	1:1625:A:MET:HE3	1:1624:A:PRO:HA	13	0.7	0.42	0.55
(1,11)	1:1625:A:MET:HE2	1:1626:A:LEU:HA	13	0.7	0.42	0.55
(1,11)	1:1625:A:MET:HE2	1:1624:A:PRO:HA	13	0.7	0.42	0.55
(1,11)	1:1625:A:MET:HE1	1:1624:A:PRO:HA	13	0.7	0.42	0.55
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	13	0.69	0.11	0.68
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	13	0.69	0.27	0.63
(1,263)	2:56:B:LEU:HD22	2:53:B:LEU:HB3	13	0.69	0.27	0.63
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HD22	13	0.69	0.27	0.63
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HB3	13	0.69	0.27	0.63
(1,263)	2:56:B:LEU:HD13	2:53:B:LEU:HD22	13	0.69	0.27	0.63
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE1	13	0.58	0.31	0.61
(1,3002)	2:42:B:ILE:HD11	2:28:B:PHE:HE2	13	0.58	0.31	0.61
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE2	13	0.58	0.31	0.61
(1,3002)	2:42:B:ILE:HD12	2:28:B:PHE:HE2	13	0.58	0.31	0.61
(1,3002)	2:42:B:ILE:HD12	2:28:B:PHE:HE1	13	0.58	0.31	0.61
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG21	13	0.58	0.35	0.5
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG22	13	0.58	0.35	0.5
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	13	0.58	0.35	0.5
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG21	13	0.58	0.35	0.5
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG23	13	0.58	0.35	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG23	13	0.58	0.35	0.5
(1,125)	1:1591:A:VAL:HG21	1:1592:A:TYR:HB3	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG23	1:1582:A:ARG:HD2	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG22	1:1582:A:ARG:HD2	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG22	1:1592:A:TYR:HB3	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD2	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD3	13	0.57	0.2	0.66
(1,125)	1:1591:A:VAL:HG23	1:1582:A:ARG:HD3	13	0.57	0.2	0.66
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	13	0.52	0.5	0.25
(1,59)	1:1590:A:LEU:HD21	1:1578:A:ASN:HB2	13	0.52	0.5	0.25
(1,59)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	13	0.52	0.5	0.25
(1,59)	1:1590:A:LEU:HD23	1:1578:A:ASN:HB2	13	0.52	0.5	0.25
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	13	0.45	0.14	0.5
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	13	0.4	0.1	0.44
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	13	0.4	0.1	0.44
(1,1020)	1:1625:A:MET:HE1	1:1625:A:MET:HG2	13	0.39	0.01	0.39
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	13	0.39	0.01	0.39
(1,1020)	1:1625:A:MET:HE3	1:1625:A:MET:HG2	13	0.39	0.01	0.39
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	13	0.38	0.07	0.41
(1,2215)	1:1644:A:LEU:HD11	1:1528:A:ASP:H	13	0.35	0.1	0.39
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	13	0.35	0.1	0.39
(1,2215)	1:1644:A:LEU:HD12	1:1528:A:ASP:H	13	0.35	0.1	0.39
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG23	13	0.35	0.15	0.31
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG22	13	0.35	0.15	0.31
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG23	13	0.35	0.15	0.31
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG22	13	0.35	0.15	0.31
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG21	13	0.35	0.15	0.31
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG21	13	0.35	0.15	0.31
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	13	0.33	0.18	0.3
(1,260)	2:32:B:ALA:H	2:38:B:ARG:HB3	13	0.33	0.18	0.3
(1,2295)	2:17:B:LEU:HD23	2:56:B:LEU:HA	13	0.28	0.11	0.28
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	13	0.28	0.11	0.28
(1,2295)	2:17:B:LEU:HD22	2:56:B:LEU:HA	13	0.28	0.11	0.28
(1,17)	1:1577:A:ALA:HB1	1:1553:A:CYS:H	13	0.28	0.12	0.26
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	13	0.28	0.12	0.26
(1,17)	1:1577:A:ALA:HB2	1:1553:A:CYS:H	13	0.28	0.12	0.26
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	13	0.28	0.11	0.26
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	13	0.28	0.11	0.26
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG22	13	0.28	0.11	0.26
(1,751)	1:1635:A:THR:HG23	1:1607:A:LYS:HD3	13	0.27	0.13	0.23
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	13	0.27	0.13	0.23
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	13	0.27	0.13	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	13	0.26	0.1	0.23
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	13	0.23	0.08	0.23
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	13	0.23	0.08	0.23
(1,1137)	1:1590:A:LEU:HD11	1:1554:A:GLY:H	13	0.23	0.08	0.23
(1,332)	2:55:B:LEU:HD13	2:56:B:LEU:H	13	0.22	0.06	0.23
(1,332)	2:55:B:LEU:HD11	2:56:B:LEU:H	13	0.22	0.06	0.23
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	13	0.22	0.06	0.23
(1,332)	2:55:B:LEU:HD11	2:42:B:ILE:H	13	0.22	0.06	0.23
(1,332)	2:55:B:LEU:HD13	2:42:B:ILE:H	13	0.22	0.06	0.23
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	13	0.22	0.04	0.21
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	13	0.12	0.01	0.12
(1,459)	1:1627:A:ILE:HG23	1:1627:A:ILE:H	13	0.12	0.01	0.12
(1,459)	1:1627:A:ILE:HG22	1:1627:A:ILE:H	13	0.12	0.01	0.12
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	13	0.11	0.01	0.11
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	12	0.96	0.41	0.99
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	12	0.96	0.41	0.99
(1,663)	1:1563:A:VAL:HG23	1:1559:A:CYS:HB2	12	0.96	0.41	0.99
(1,49)	1:1565:A:ALA:HB3	1:1556:A:ASN:HB3	12	0.82	0.48	0.71
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	12	0.82	0.48	0.71
(1,49)	1:1540:A:ALA:HB1	1:1625:A:MET:HG2	12	0.82	0.48	0.71
(1,49)	1:1540:A:ALA:HB2	1:1625:A:MET:HG2	12	0.82	0.48	0.71
(1,49)	1:1565:A:ALA:HB1	1:1556:A:ASN:HB3	12	0.82	0.48	0.71
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	12	0.6	0.33	0.52
(1,693)	1:1590:A:LEU:HD21	1:1592:A:TYR:HA	12	0.6	0.18	0.62
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	12	0.6	0.18	0.62
(1,693)	1:1590:A:LEU:HD23	1:1592:A:TYR:HA	12	0.6	0.18	0.62
(1,287)	2:64:B:ALA:HA	2:63:B:PRO:HB3	12	0.58	0.3	0.52
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	12	0.58	0.3	0.52
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	12	0.53	0.26	0.48
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	12	0.53	0.26	0.48
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	12	0.53	0.26	0.48
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	12	0.52	0.21	0.54
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD2	12	0.52	0.21	0.54
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	12	0.51	0.02	0.5
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	12	0.46	0.23	0.42
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG21	12	0.44	0.18	0.56
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	12	0.44	0.18	0.56
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	12	0.44	0.18	0.56
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	12	0.41	0.16	0.38
(1,2273)	2:14:B:VAL:HG21	2:26:B:PHE:HB2	12	0.41	0.12	0.42
(1,2273)	2:14:B:VAL:HG23	2:26:B:PHE:HB2	12	0.41	0.12	0.42
(1,2273)	2:14:B:VAL:HG22	2:26:B:PHE:HB2	12	0.41	0.12	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2273)	2:14:B:VAL:HG12	2:26:B:PHE:HB2	12	0.41	0.12	0.42
(1,933)	1:1626:A:LEU:HD13	1:1636:A:LEU:HG	12	0.39	0.03	0.38
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	12	0.39	0.03	0.38
(1,933)	1:1626:A:LEU:HD12	1:1636:A:LEU:HG	12	0.39	0.03	0.38
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	12	0.39	0.09	0.42
(1,1837)	1:1618:A:ALA:HB1	1:1622:A:ASN:HD22	12	0.34	0.07	0.34
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	12	0.34	0.07	0.34
(1,1837)	1:1618:A:ALA:HB2	1:1622:A:ASN:HD22	12	0.34	0.07	0.34
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG22	12	0.33	0.13	0.32
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG21	12	0.33	0.13	0.32
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG23	12	0.33	0.13	0.32
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	12	0.3	0.12	0.36
(1,983)	1:1580:A:ARG:HD3	1:1580:A:ARG:HA	12	0.3	0.12	0.36
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG22	12	0.26	0.06	0.28
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG21	12	0.26	0.06	0.28
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG23	12	0.26	0.06	0.28
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	12	0.23	0.08	0.22
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD22	12	0.23	0.08	0.22
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD23	12	0.23	0.08	0.22
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	12	0.2	0.05	0.22
(1,1139)	1:1577:A:ALA:HB2	1:1554:A:GLY:H	12	0.16	0.03	0.17
(1,1139)	1:1577:A:ALA:HB1	1:1554:A:GLY:H	12	0.16	0.03	0.17
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	12	0.16	0.03	0.17
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	12	0.11	0.02	0.11
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	11	1.14	0.12	1.16
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG11	11	1.14	0.12	1.16
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG12	11	1.14	0.12	1.16
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	11	0.9	0.88	0.34
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD21	11	0.9	0.88	0.34
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD22	11	0.9	0.88	0.34
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD11	11	0.86	0.31	0.82
(1,619)	1:1626:A:LEU:HD23	1:1629:A:LEU:HD12	11	0.86	0.31	0.82
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD13	11	0.86	0.31	0.82
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD22	11	0.86	0.31	0.82
(1,619)	1:1626:A:LEU:HD21	1:1629:A:LEU:HD12	11	0.86	0.31	0.82
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD12	11	0.86	0.31	0.82
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG13	11	0.84	0.33	0.71
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG11	11	0.84	0.33	0.71
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG12	11	0.84	0.33	0.71
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	11	0.79	0.44	0.9
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD22	11	0.68	0.96	0.41
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	11	0.68	0.96	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD23	11	0.68	0.96	0.41
(1,2445)	2:7:B:THR:HG22	2:50:B:SER:HB3	11	0.66	0.23	0.67
(1,2445)	2:7:B:THR:HG23	2:50:B:SER:HB3	11	0.66	0.23	0.67
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	11	0.66	0.23	0.67
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG13	11	0.66	0.23	0.79
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG12	11	0.66	0.23	0.79
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	11	0.66	0.23	0.79
(1,40)	1:1587:A:VAL:HG22	1:1586:A:GLN:HE21	11	0.64	0.29	0.65
(1,40)	1:1587:A:VAL:HG21	1:1589:A:GLN:HE21	11	0.64	0.29	0.65
(1,40)	1:1587:A:VAL:HG23	1:1586:A:GLN:HE21	11	0.64	0.29	0.65
(1,40)	1:1587:A:VAL:HG21	1:1586:A:GLN:HE21	11	0.64	0.29	0.65
(1,2322)	2:32:B:ALA:HB1	2:33:B:SER:HB3	11	0.63	0.38	0.55
(1,2322)	2:32:B:ALA:HB3	2:33:B:SER:HB3	11	0.63	0.38	0.55
(1,2322)	2:32:B:ALA:HB2	2:33:B:SER:HB3	11	0.63	0.38	0.55
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB1	11	0.59	0.11	0.59
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	11	0.59	0.11	0.59
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB3	11	0.59	0.11	0.59
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	11	0.56	0.03	0.56
(1,1299)	1:1563:A:VAL:HG22	1:1563:A:VAL:H	11	0.56	0.03	0.56
(1,1299)	1:1563:A:VAL:HG21	1:1563:A:VAL:H	11	0.56	0.03	0.56
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	11	0.42	0.16	0.38
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	11	0.42	0.29	0.34
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG21	11	0.41	0.17	0.42
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG13	11	0.41	0.17	0.42
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG22	11	0.41	0.17	0.42
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG12	11	0.41	0.17	0.42
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG23	11	0.41	0.17	0.42
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG22	11	0.41	0.17	0.42
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	11	0.36	0.16	0.32
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG11	11	0.36	0.16	0.32
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG12	11	0.36	0.16	0.32
(1,1228)	1:1642:A:THR:HG21	1:1640:A:TRP:HE1	11	0.33	0.13	0.25
(1,1228)	1:1642:A:THR:HG23	1:1640:A:TRP:HE1	11	0.33	0.13	0.25
(1,1228)	1:1642:A:THR:HG22	1:1640:A:TRP:HE1	11	0.33	0.13	0.25
(1,483)	1:1610:A:ILE:HG23	1:1590:A:LEU:HB3	11	0.3	0.14	0.28
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	11	0.3	0.14	0.28
(1,483)	1:1610:A:ILE:HG21	1:1590:A:LEU:HB3	11	0.3	0.14	0.28
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	11	0.26	0.12	0.22
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	11	0.2	0.09	0.15
(1,354)	1:1606:A:TYR:HD2	2:19:B:PHE:HZ	11	0.2	0.09	0.15
(1,354)	2:38:B:ARG:HE	2:59:B:TYR:HE2	11	0.2	0.09	0.15
(1,1638)	1:1645:A:ALA:HB2	1:1646:A:CYS:H	11	0.19	0.07	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	11	0.19	0.07	0.2
(1,1638)	1:1645:A:ALA:HB1	1:1646:A:CYS:H	11	0.19	0.07	0.2
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	11	0.17	0.05	0.17
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	11	0.15	0.02	0.15
(1,443)	1:1550:A:MET:HE1	1:1550:A:MET:H	11	0.15	0.02	0.15
(1,443)	1:1550:A:MET:HE3	1:1550:A:MET:H	11	0.15	0.02	0.15
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	11	0.15	0.01	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	11	0.15	0.01	0.14
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	10	1.3	1.38	0.5
(1,2504)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	10	1.3	1.38	0.5
(1,2504)	2:13:B:LEU:HD23	2:9:B:CYS:HB3	10	1.3	1.38	0.5
(1,1089)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	10	1.1	1.12	0.56
(1,1089)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	10	1.1	1.12	0.56
(1,1089)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	10	1.1	1.12	0.56
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	10	1.03	0.53	1.08
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD22	10	0.92	0.85	0.62
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD23	10	0.92	0.85	0.62
(1,3009)	2:56:B:LEU:HD21	2:17:B:LEU:HD23	10	0.92	0.85	0.62
(1,3009)	2:56:B:LEU:HD21	2:17:B:LEU:HD21	10	0.92	0.85	0.62
(1,3009)	2:42:B:ILE:HG23	2:17:B:LEU:HD21	10	0.92	0.85	0.62
(1,3009)	2:56:B:LEU:HD23	2:17:B:LEU:HD23	10	0.92	0.85	0.62
(1,325)	2:17:B:LEU:HD11	2:28:B:PHE:HB2	10	0.91	0.24	0.83
(1,325)	2:17:B:LEU:HD12	2:28:B:PHE:HB2	10	0.91	0.24	0.83
(1,325)	2:17:B:LEU:HD12	2:14:B:VAL:HA	10	0.91	0.24	0.83
(1,325)	2:17:B:LEU:HD13	2:28:B:PHE:HB2	10	0.91	0.24	0.83
(1,325)	2:17:B:LEU:HD11	2:14:B:VAL:HA	10	0.91	0.24	0.83
(1,691)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	10	0.89	1.12	0.34
(1,691)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	10	0.89	1.12	0.34
(1,691)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	10	0.89	1.12	0.34
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	10	0.66	0.09	0.64
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD11	10	0.66	0.82	0.48
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD13	10	0.66	0.82	0.48
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD12	10	0.66	0.82	0.48
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD11	10	0.66	0.82	0.48
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	10	0.66	0.82	0.48
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD13	10	0.66	0.82	0.48
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	10	0.63	0.68	0.38
(1,230)	2:55:B:LEU:HD11	2:59:B:TYR:H	10	0.63	0.68	0.38
(1,230)	2:55:B:LEU:HD13	2:59:B:TYR:H	10	0.63	0.68	0.38
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	10	0.62	0.06	0.62
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	10	0.59	0.37	0.45
(1,1033)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	10	0.58	0.23	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1033)	1:1645:A:ALA:HB1	1:1614:A:CYS:HB3	10	0.58	0.23	0.55
(1,1033)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	10	0.58	0.23	0.55
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD22	10	0.56	0.26	0.64
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD21	10	0.56	0.26	0.64
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD23	10	0.56	0.26	0.64
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	10	0.54	0.15	0.57
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG13	10	0.54	0.15	0.57
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG12	10	0.54	0.15	0.57
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	10	0.53	0.3	0.46
(1,440)	1:1550:A:MET:HE3	1:1638:A:PHE:HD2	10	0.52	0.21	0.55
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD2	10	0.52	0.21	0.55
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD1	10	0.52	0.21	0.55
(1,440)	1:1550:A:MET:HE3	1:1638:A:PHE:HD1	10	0.52	0.21	0.55
(1,440)	1:1550:A:MET:HE2	1:1638:A:PHE:HD1	10	0.52	0.21	0.55
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	10	0.52	0.21	0.55
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB1	10	0.52	0.21	0.55
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB3	10	0.52	0.21	0.55
(1,523)	1:1613:A:VAL:HG21	1:1641:A:HIS:HD2	10	0.51	0.13	0.56
(1,523)	1:1613:A:VAL:HG22	1:1641:A:HIS:HD2	10	0.51	0.13	0.56
(1,523)	1:1613:A:VAL:HG23	1:1641:A:HIS:HD2	10	0.51	0.13	0.56
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	10	0.5	0.05	0.51
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	10	0.46	0.06	0.48
(1,722)	1:1581:A:LEU:HD13	1:1518:A:VAL:HB	10	0.45	0.8	0.2
(1,722)	1:1581:A:LEU:HD11	1:1518:A:VAL:HB	10	0.45	0.8	0.2
(1,722)	1:1581:A:LEU:HD12	1:1518:A:VAL:HB	10	0.45	0.8	0.2
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	10	0.4	0.35	0.26
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	10	0.4	0.11	0.4
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	10	0.38	0.14	0.36
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD2	10	0.38	0.14	0.36
(1,668)	1:1635:A:THR:HG22	1:1607:A:LYS:HG3	10	0.38	0.16	0.34
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	10	0.38	0.16	0.34
(1,668)	1:1635:A:THR:HG23	1:1607:A:LYS:HG3	10	0.38	0.16	0.34
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	10	0.37	0.19	0.32
(1,266)	2:62:B:THR:HG23	2:63:B:PRO:HG3	10	0.37	0.15	0.32
(1,266)	2:62:B:THR:HG21	2:63:B:PRO:HG3	10	0.37	0.15	0.32
(1,266)	2:62:B:THR:HG23	2:24:B:ARG:HG3	10	0.37	0.15	0.32
(1,266)	2:62:B:THR:HG22	2:24:B:ARG:HG3	10	0.37	0.15	0.32
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	10	0.36	0.19	0.3
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE1	10	0.34	0.13	0.38
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE2	10	0.34	0.13	0.38
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	10	0.34	0.13	0.38
(1,442)	1:1550:A:MET:HE2	1:1640:A:TRP:HB2	10	0.33	0.11	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,442)	1:1550:A:MET:HE1	1:1640:A:TRP:HB2	10	0.33	0.11	0.34
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	10	0.33	0.11	0.34
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG3	10	0.31	0.15	0.28
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	10	0.31	0.15	0.28
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	10	0.3	0.13	0.3
(1,1108)	1:1583:A:TYR:HD1	1:1585:A:ASP:HA	10	0.3	0.13	0.3
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	10	0.28	0.04	0.26
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD2	10	0.28	0.04	0.26
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	10	0.27	0.1	0.26
(1,300)	2:36:B:SER:H	2:32:B:ALA:HB2	10	0.27	0.1	0.26
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,441)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,441)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,446)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,446)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	10	0.26	0.02	0.26
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG22	10	0.26	0.12	0.26
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG23	10	0.26	0.12	0.26
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG21	10	0.26	0.12	0.26
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	10	0.26	0.1	0.26
(1,203)	1:1598:A:CYS:H	1:1603:A:GLY:HA2	10	0.26	0.1	0.26
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	10	0.24	0.1	0.2
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	10	0.24	0.1	0.2
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	10	0.22	0.12	0.19
(1,2)	1:1552:A:ILE:HD11	1:1592:A:TYR:HD2	10	0.22	0.12	0.19
(1,2)	1:1552:A:ILE:HD13	1:1592:A:TYR:HD2	10	0.22	0.12	0.19
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	10	0.16	0.03	0.16
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD22	9	0.73	0.39	0.98
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	9	0.73	0.39	0.98
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD23	9	0.73	0.39	0.98
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD13	9	0.69	0.29	0.6
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD11	9	0.69	0.29	0.6
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG22	9	0.69	0.29	0.6
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG23	9	0.69	0.29	0.6
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG21	9	0.69	0.29	0.6
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD12	9	0.69	0.29	0.6
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG11	9	0.66	0.02	0.66
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	9	0.66	0.02	0.66
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG13	9	0.66	0.02	0.66
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD23	9	0.65	0.52	0.37
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD22	9	0.65	0.52	0.37
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD21	9	0.65	0.52	0.37

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,536)	1:1609:A:VAL:HG23	1:1607:A:LYS:HE3	9	0.64	0.37	0.7
(1,536)	1:1609:A:VAL:HG22	1:1607:A:LYS:HE3	9	0.64	0.37	0.7
(1,536)	1:1609:A:VAL:HG21	1:1607:A:LYS:HE3	9	0.64	0.37	0.7
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD11	9	0.61	0.37	0.58
(1,932)	1:1601:A:LYS:HD3	1:1604:A:LEU:HD13	9	0.61	0.37	0.58
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD13	9	0.61	0.37	0.58
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD21	9	0.61	0.37	0.58
(1,248)	2:29:B:SER:HB3	2:30:B:ARG:HG3	9	0.59	0.29	0.54
(1,248)	2:29:B:SER:HB3	2:30:B:ARG:HG2	9	0.59	0.29	0.54
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG2	9	0.59	0.29	0.54
(1,248)	2:32:B:ALA:HB3	2:39:B:SER:HB3	9	0.59	0.29	0.54
(1,248)	2:36:B:SER:HB2	2:30:B:ARG:HG3	9	0.59	0.29	0.54
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG3	9	0.59	0.29	0.54
(1,248)	2:36:B:SER:HB3	2:30:B:ARG:HG2	9	0.59	0.29	0.54
(1,646)	1:1529:A:LEU:HD11	1:1612:A:PHE:HZ	9	0.54	1.07	0.16
(1,646)	1:1529:A:LEU:HD12	1:1612:A:PHE:HZ	9	0.54	1.07	0.16
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	9	0.54	1.07	0.16
(1,1753)	1:1604:A:LEU:HD21	1:1605:A:SER:H	9	0.53	0.22	0.47
(1,1753)	1:1604:A:LEU:HD22	1:1605:A:SER:H	9	0.53	0.22	0.47
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD13	9	0.53	0.22	0.47
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD12	9	0.53	0.22	0.47
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD11	9	0.53	0.22	0.47
(1,1753)	1:1604:A:LEU:HD23	1:1605:A:SER:H	9	0.53	0.22	0.47
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	9	0.51	0.57	0.34
(1,614)	1:1626:A:LEU:HD21	1:1636:A:LEU:HB2	9	0.51	0.57	0.34
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG11	9	0.47	0.05	0.46
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	9	0.47	0.05	0.46
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG13	9	0.47	0.05	0.46
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD23	9	0.44	0.24	0.46
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD22	9	0.44	0.24	0.46
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	9	0.44	0.24	0.46
(1,396)	1:1542:A:TYR:HD2	2:19:B:PHE:HD1	9	0.4	0.14	0.41
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	9	0.4	0.14	0.41
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	9	0.37	0.33	0.27
(1,724)	1:1581:A:LEU:HD22	1:1588:A:LEU:HA	9	0.36	0.11	0.37
(1,724)	1:1581:A:LEU:HD21	1:1588:A:LEU:HA	9	0.36	0.11	0.37
(1,724)	1:1581:A:LEU:HD23	1:1588:A:LEU:HA	9	0.36	0.11	0.37
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG23	9	0.36	0.15	0.41
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG21	9	0.36	0.15	0.41
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG22	9	0.36	0.15	0.41
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD11	9	0.35	0.14	0.41
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD23	9	0.35	0.14	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD12	9	0.35	0.14	0.41
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	9	0.35	0.16	0.4
(1,246)	2:36:B:SER:HB2	2:33:B:SER:H	9	0.35	0.16	0.4
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	9	0.34	0.04	0.33
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	9	0.34	0.17	0.33
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	9	0.34	0.12	0.35
(1,1114)	1:1583:A:TYR:HE1	1:1585:A:ASP:HA	9	0.34	0.12	0.35
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD3	9	0.33	0.09	0.34
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	9	0.33	0.09	0.34
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	9	0.33	0.18	0.26
(1,2324)	2:64:B:ALA:HB1	2:63:B:PRO:HA	9	0.32	0.14	0.29
(1,2324)	2:64:B:ALA:HB2	2:63:B:PRO:HA	9	0.32	0.14	0.29
(1,2324)	2:64:B:ALA:HB3	2:63:B:PRO:HA	9	0.32	0.14	0.29
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB1	9	0.3	0.13	0.25
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB2	9	0.3	0.13	0.25
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB3	9	0.3	0.13	0.25
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	9	0.3	0.11	0.36
(1,653)	1:1563:A:VAL:HG21	1:1565:A:ALA:H	9	0.29	0.03	0.31
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	9	0.29	0.03	0.31
(1,653)	1:1563:A:VAL:HG22	1:1565:A:ALA:H	9	0.29	0.03	0.31
(1,583)	1:1540:A:ALA:HB3	1:1638:A:PHE:HE1	9	0.27	0.14	0.22
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE1	9	0.27	0.14	0.22
(1,583)	1:1540:A:ALA:HB1	1:1638:A:PHE:HE1	9	0.27	0.14	0.22
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE2	9	0.27	0.14	0.22
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG22	9	0.25	0.11	0.22
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG23	9	0.25	0.11	0.22
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG13	9	0.25	0.11	0.22
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG12	9	0.25	0.11	0.22
(1,1774)	1:1563:A:VAL:HG21	1:1564:A:GLY:H	9	0.24	0.02	0.23
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	9	0.24	0.02	0.23
(1,1774)	1:1563:A:VAL:HG22	1:1564:A:GLY:H	9	0.24	0.02	0.23
(1,599)	1:1587:A:VAL:HG13	1:1611:A:SER:HB2	9	0.23	0.09	0.24
(1,599)	1:1587:A:VAL:HG12	1:1611:A:SER:HB2	9	0.23	0.09	0.24
(1,599)	1:1587:A:VAL:HG11	1:1611:A:SER:HB2	9	0.23	0.09	0.24
(1,1927)	1:1563:A:VAL:HG21	1:1575:A:GLY:H	9	0.21	0.02	0.21
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	9	0.21	0.02	0.21
(1,1927)	1:1563:A:VAL:HG22	1:1575:A:GLY:H	9	0.21	0.02	0.21
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD1	9	0.2	0.09	0.18
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	9	0.2	0.09	0.18
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG11	9	0.19	0.06	0.17
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG12	9	0.19	0.06	0.17
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG13	9	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	9	0.19	0.04	0.19
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD3	9	0.19	0.04	0.19
(1,2147)	1:1591:A:VAL:HG21	1:1610:A:ILE:H	9	0.18	0.05	0.18
(1,2147)	1:1591:A:VAL:HG23	1:1610:A:ILE:H	9	0.18	0.05	0.18
(1,2147)	1:1591:A:VAL:HG22	1:1610:A:ILE:H	9	0.18	0.05	0.18
(1,467)	1:1625:A:MET:HE3	1:1625:A:MET:HA	9	0.15	0.03	0.16
(1,467)	1:1625:A:MET:HE2	1:1625:A:MET:HA	9	0.15	0.03	0.16
(1,467)	1:1625:A:MET:HE1	1:1625:A:MET:HA	9	0.15	0.03	0.16
(1,638)	1:1588:A:LEU:HD21	1:1588:A:LEU:HB2	9	0.13	0.01	0.13
(1,638)	1:1588:A:LEU:HD22	1:1588:A:LEU:HB2	9	0.13	0.01	0.13
(1,638)	1:1588:A:LEU:HD23	1:1588:A:LEU:HB2	9	0.13	0.01	0.13
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	9	0.12	0.01	0.12
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	8	1.14	0.52	1.3
(1,1040)	1:1591:A:VAL:HG23	1:1607:A:LYS:HD3	8	1.14	0.52	1.3
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	8	1.09	0.68	1.48
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	8	0.88	0.2	0.88
(1,2315)	2:43:B:VAL:HG23	2:40:B:ARG:HD2	8	0.87	0.85	0.62
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD3	8	0.87	0.85	0.62
(1,2315)	2:43:B:VAL:HG22	2:40:B:ARG:HD3	8	0.87	0.85	0.62
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD2	8	0.87	0.85	0.62
(1,2529)	2:43:B:VAL:HG22	2:44:B:GLU:HG3	8	0.81	0.64	0.68
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	8	0.81	0.64	0.68
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD11	8	0.75	0.11	0.71
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	8	0.75	0.11	0.71
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	8	0.75	0.11	0.71
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	8	0.69	0.16	0.66
(1,124)	1:1613:A:VAL:HG21	1:1611:A:SER:HB2	8	0.69	0.16	0.66
(1,124)	1:1613:A:VAL:HG23	1:1611:A:SER:HB2	8	0.69	0.16	0.66
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE2	8	0.64	0.22	0.72
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE1	8	0.64	0.22	0.72
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE2	8	0.64	0.22	0.72
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE1	8	0.64	0.22	0.72
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	8	0.63	0.4	0.55
(1,2321)	2:32:B:ALA:HB2	2:33:B:SER:HA	8	0.62	0.3	0.62
(1,2321)	2:32:B:ALA:HB2	2:36:B:SER:HA	8	0.62	0.3	0.62
(1,2321)	2:32:B:ALA:HB3	2:33:B:SER:HA	8	0.62	0.3	0.62
(1,2321)	2:32:B:ALA:HB3	2:36:B:SER:HA	8	0.62	0.3	0.62
(1,2321)	2:32:B:ALA:HB1	2:33:B:SER:HA	8	0.62	0.3	0.62
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	8	0.55	0.08	0.52
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	8	0.48	0.03	0.48
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG12	8	0.46	0.05	0.48
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG13	8	0.46	0.05	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG11	8	0.46	0.05	0.48
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD23	8	0.46	0.28	0.43
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	8	0.46	0.28	0.43
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD22	8	0.46	0.28	0.43
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	8	0.45	0.16	0.44
(1,2441)	2:8:B:LEU:HD11	2:8:B:LEU:HA	8	0.45	0.16	0.44
(1,2441)	2:8:B:LEU:HD13	2:8:B:LEU:HA	8	0.45	0.16	0.44
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	8	0.45	0.14	0.5
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	8	0.44	0.74	0.16
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD11	8	0.44	0.74	0.16
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	8	0.42	0.04	0.43
(1,1056)	1:1626:A:LEU:HD13	1:1636:A:LEU:HB3	8	0.41	0.03	0.42
(1,1056)	1:1626:A:LEU:HD11	1:1636:A:LEU:HB3	8	0.41	0.03	0.42
(1,1056)	1:1626:A:LEU:HD12	1:1636:A:LEU:HB3	8	0.41	0.03	0.42
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	8	0.41	0.02	0.4
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG12	8	0.39	0.14	0.42
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG11	8	0.39	0.14	0.42
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG13	8	0.39	0.14	0.42
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	8	0.36	0.11	0.33
(1,2376)	2:42:B:ILE:HG21	2:28:B:PHE:HB3	8	0.34	0.16	0.37
(1,2376)	2:42:B:ILE:HG22	2:28:B:PHE:HB3	8	0.34	0.16	0.37
(1,2376)	2:42:B:ILE:HG23	2:28:B:PHE:HB3	8	0.34	0.16	0.37
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	8	0.33	0.11	0.36
(1,727)	1:1629:A:LEU:HD21	1:1631:A:LYS:HA	8	0.33	0.11	0.36
(1,727)	1:1629:A:LEU:HD22	1:1631:A:LYS:HA	8	0.33	0.11	0.36
(1,2067)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	8	0.33	0.23	0.28
(1,2067)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	8	0.33	0.23	0.28
(1,2067)	1:1590:A:LEU:HD23	1:1578:A:ASN:H	8	0.33	0.23	0.28
(1,1495)	1:1563:A:VAL:HG21	1:1574:A:VAL:H	8	0.31	0.03	0.32
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	8	0.31	0.03	0.32
(1,1495)	1:1563:A:VAL:HG22	1:1574:A:VAL:H	8	0.31	0.03	0.32
(1,1323)	1:1563:A:VAL:HG21	1:1577:A:ALA:H	8	0.29	0.1	0.32
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	8	0.29	0.1	0.32
(1,1323)	1:1563:A:VAL:HG22	1:1577:A:ALA:H	8	0.29	0.1	0.32
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	8	0.29	0.05	0.27
(1,97)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	8	0.28	0.13	0.24
(1,97)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	8	0.28	0.13	0.24
(1,97)	1:1590:A:LEU:HD23	1:1578:A:ASN:H	8	0.28	0.13	0.24
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	8	0.27	0.13	0.26
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	8	0.26	0.14	0.2
(1,208)	1:1609:A:VAL:HG12	1:1590:A:LEU:H	8	0.26	0.14	0.2
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	8	0.25	0.09	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	8	0.22	0.06	0.24
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE2	8	0.22	0.06	0.24
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG22	8	0.2	0.08	0.18
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG21	8	0.2	0.08	0.18
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG23	8	0.2	0.08	0.18
(1,581)	1:1532:A:LEU:HD21	1:1532:A:LEU:H	8	0.2	0.1	0.15
(1,581)	1:1532:A:LEU:HD23	1:1532:A:LEU:H	8	0.2	0.1	0.15
(1,581)	1:1532:A:LEU:HD22	1:1532:A:LEU:H	8	0.2	0.1	0.15
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	8	0.2	0.08	0.16
(1,1405)	1:1539:A:THR:HG22	1:1540:A:ALA:H	8	0.19	0.08	0.16
(1,1405)	1:1539:A:THR:HG23	1:1540:A:ALA:H	8	0.19	0.08	0.16
(1,1405)	1:1539:A:THR:HG21	1:1540:A:ALA:H	8	0.19	0.08	0.16
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG12	8	0.19	0.07	0.18
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG13	8	0.19	0.07	0.18
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG11	8	0.19	0.07	0.18
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	8	0.19	0.07	0.18
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	8	0.18	0.03	0.18
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	8	0.18	0.03	0.18
(1,144)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	8	0.18	0.06	0.17
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	8	0.18	0.06	0.17
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	8	0.15	0.04	0.14
(1,631)	1:1539:A:THR:HG21	1:1549:A:TYR:HA	8	0.12	0.01	0.12
(1,631)	1:1539:A:THR:HG23	1:1549:A:TYR:HA	8	0.12	0.01	0.12
(1,631)	1:1539:A:THR:HG22	1:1549:A:TYR:HA	8	0.12	0.01	0.12
(1,1214)	1:1625:A:MET:HE1	1:1641:A:HIS:H	7	0.99	0.04	0.99
(1,1214)	1:1625:A:MET:HE3	1:1641:A:HIS:H	7	0.99	0.04	0.99
(1,2846)	2:17:B:LEU:HD13	2:26:B:PHE:HD2	7	0.97	0.48	1.07
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD2	7	0.97	0.48	1.07
(1,2846)	2:17:B:LEU:HD12	2:26:B:PHE:HD1	7	0.97	0.48	1.07
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD1	7	0.97	0.48	1.07
(1,2846)	2:17:B:LEU:HD12	2:26:B:PHE:HD2	7	0.97	0.48	1.07
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	7	0.79	0.02	0.8
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	7	0.75	0.04	0.75
(1,79)	1:1632:A:GLN:HG3	1:1631:A:LYS:H	7	0.75	0.04	0.75
(1,2860)	2:17:B:LEU:HD11	2:28:B:PHE:HE2	7	0.71	0.37	0.78
(1,2860)	2:17:B:LEU:HD13	2:28:B:PHE:HE2	7	0.71	0.37	0.78
(1,2860)	2:17:B:LEU:HD11	2:28:B:PHE:HE1	7	0.71	0.37	0.78
(1,2860)	2:17:B:LEU:HD13	2:28:B:PHE:HE1	7	0.71	0.37	0.78
(1,2860)	2:17:B:LEU:HD12	2:28:B:PHE:HE1	7	0.71	0.37	0.78
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD1	7	0.68	0.34	0.56
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD2	7	0.68	0.34	0.56
(1,2259)	2:42:B:ILE:HG23	2:28:B:PHE:HD1	7	0.68	0.34	0.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	7	0.65	0.15	0.64
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	7	0.5	0.28	0.36
(1,25)	1:1584:A:VAL:HG11	1:1582:A:ARG:HD2	7	0.5	0.25	0.34
(1,25)	1:1584:A:VAL:HG12	1:1582:A:ARG:HD3	7	0.5	0.25	0.34
(1,25)	1:1591:A:VAL:HG13	1:1582:A:ARG:HD3	7	0.5	0.25	0.34
(1,25)	1:1591:A:VAL:HG12	1:1582:A:ARG:HD3	7	0.5	0.25	0.34
(1,25)	1:1584:A:VAL:HG13	1:1582:A:ARG:HD3	7	0.5	0.25	0.34
(1,25)	1:1584:A:VAL:HG11	1:1582:A:ARG:HD3	7	0.5	0.25	0.34
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG3	7	0.5	0.12	0.56
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG2	7	0.5	0.12	0.56
(1,142)	1:1581:A:LEU:HD11	1:1582:A:ARG:HG3	7	0.49	0.77	0.21
(1,142)	1:1581:A:LEU:HD13	1:1582:A:ARG:HG3	7	0.49	0.77	0.21
(1,142)	1:1581:A:LEU:HD12	1:1582:A:ARG:HG3	7	0.49	0.77	0.21
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD23	7	0.48	0.29	0.42
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD22	7	0.48	0.29	0.42
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD21	7	0.48	0.29	0.42
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	7	0.45	0.04	0.45
(1,745)	1:1601:A:LYS:HD2	1:1601:A:LYS:HA	7	0.44	0.14	0.44
(1,745)	1:1601:A:LYS:HD3	1:1601:A:LYS:HA	7	0.44	0.14	0.44
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD1	7	0.43	0.13	0.48
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD2	7	0.43	0.13	0.48
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG13	7	0.41	0.3	0.19
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	7	0.41	0.3	0.19
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG12	7	0.41	0.3	0.19
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	7	0.39	0.08	0.43
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	7	0.39	0.05	0.4
(1,424)	1:1552:A:ILE:HD11	1:1592:A:TYR:HH	7	0.37	0.19	0.33
(1,424)	1:1552:A:ILE:HD12	1:1592:A:TYR:HH	7	0.37	0.19	0.33
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	7	0.34	0.17	0.26
(1,1915)	1:1618:A:ALA:HB2	1:1619:A:GLY:H	7	0.34	0.17	0.26
(1,1915)	1:1618:A:ALA:HB1	1:1619:A:GLY:H	7	0.34	0.17	0.26
(1,1019)	1:1625:A:MET:HE2	1:1625:A:MET:HG3	7	0.33	0.02	0.33
(1,1019)	1:1625:A:MET:HE1	1:1625:A:MET:HG3	7	0.33	0.02	0.33
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	7	0.32	0.04	0.31
(1,2323)	2:32:B:ALA:HB3	2:33:B:SER:HB2	7	0.3	0.32	0.17
(1,2323)	2:32:B:ALA:HB1	2:33:B:SER:HB2	7	0.3	0.32	0.17
(1,2323)	2:32:B:ALA:HB3	2:36:B:SER:HB3	7	0.3	0.32	0.17
(1,2323)	2:32:B:ALA:HB2	2:33:B:SER:HB2	7	0.3	0.32	0.17
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	7	0.3	0.29	0.13
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	7	0.27	0.06	0.28
(1,411)	1:1602:A:SER:H	2:52:B:ASP:HA	7	0.27	0.1	0.31
(1,411)	1:1602:A:SER:H	1:1600:A:SER:HA	7	0.27	0.1	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	7	0.26	0.05	0.25
(1,2521)	2:35:B:VAL:HG22	2:33:B:SER:HB3	7	0.25	0.15	0.21
(1,2521)	2:35:B:VAL:HG23	2:33:B:SER:HB3	7	0.25	0.15	0.21
(1,2521)	2:35:B:VAL:HG21	2:33:B:SER:HB3	7	0.25	0.15	0.21
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	7	0.25	0.14	0.17
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB3	7	0.24	0.06	0.23
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB1	7	0.24	0.06	0.23
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB2	7	0.24	0.06	0.23
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	7	0.22	0.08	0.23
(1,420)	1:1627:A:ILE:HD12	1:1639:A:SER:HB2	7	0.22	0.07	0.21
(1,420)	1:1627:A:ILE:HD13	1:1639:A:SER:HB2	7	0.22	0.07	0.21
(1,420)	1:1627:A:ILE:HD11	1:1639:A:SER:HB2	7	0.22	0.07	0.21
(1,2373)	2:42:B:ILE:HG21	2:59:B:TYR:HD2	7	0.19	0.04	0.18
(1,2373)	2:42:B:ILE:HG22	2:59:B:TYR:HD1	7	0.19	0.04	0.18
(1,2373)	2:42:B:ILE:HG23	2:59:B:TYR:HD1	7	0.19	0.04	0.18
(1,2373)	2:42:B:ILE:HG22	2:59:B:TYR:HD2	7	0.19	0.04	0.18
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	7	0.18	0.05	0.17
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	7	0.17	0.05	0.16
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	7	0.17	0.03	0.18
(1,13)	1:1547:A:VAL:HG22	1:1548:A:VAL:HA	7	0.16	0.04	0.15
(1,13)	1:1547:A:VAL:HG23	1:1548:A:VAL:HA	7	0.16	0.04	0.15
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	7	0.16	0.01	0.16
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	7	0.16	0.05	0.16
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD2	7	0.16	0.05	0.16
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	7	0.16	0.05	0.12
(1,1451)	1:1547:A:VAL:HG12	1:1548:A:VAL:H	7	0.16	0.05	0.12
(1,1451)	1:1547:A:VAL:HG11	1:1548:A:VAL:H	7	0.16	0.05	0.12
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	7	0.14	0.03	0.12
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	7	0.12	0.02	0.13
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	7	0.11	0.01	0.11
(1,564)	1:1591:A:VAL:HG21	1:1593:A:LYS:H	6	1.3	0.7	1.79
(1,564)	1:1591:A:VAL:HG23	1:1593:A:LYS:H	6	1.3	0.7	1.79
(1,564)	1:1591:A:VAL:HG22	1:1593:A:LYS:H	6	1.3	0.7	1.79
(1,3010)	2:17:B:LEU:HD23	2:56:B:LEU:HD13	6	1.21	0.53	1.36
(1,3010)	2:17:B:LEU:HD23	2:56:B:LEU:HD12	6	1.21	0.53	1.36
(1,3010)	2:17:B:LEU:HD22	2:56:B:LEU:HD11	6	1.21	0.53	1.36
(1,3010)	2:17:B:LEU:HD21	2:56:B:LEU:HD12	6	1.21	0.53	1.36
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	6	1.08	0.47	1.32
(1,448)	1:1550:A:MET:HE1	1:1550:A:MET:HG3	6	1.08	0.06	1.1
(1,448)	1:1550:A:MET:HE2	1:1550:A:MET:HG3	6	1.08	0.06	1.1
(1,696)	1:1644:A:LEU:HD22	1:1529:A:LEU:HD23	6	1.02	1.11	0.26
(1,696)	1:1644:A:LEU:HD21	1:1529:A:LEU:HD23	6	1.02	1.11	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,696)	1:1644:A:LEU:HD23	1:1529:A:LEU:HD23	6	1.02	1.11	0.26
(1,696)	1:1644:A:LEU:HD23	1:1529:A:LEU:HD22	6	1.02	1.11	0.26
(1,372)	1:1569:A:GLN:HG2	2:15:B:ASP:HB3	6	0.9	0.19	0.82
(1,372)	1:1569:A:GLN:HG3	2:15:B:ASP:HB3	6	0.9	0.19	0.82
(1,47)	1:1518:A:VAL:HG13	1:1513:A:HIS:HB3	6	0.84	0.33	1.0
(1,47)	1:1518:A:VAL:HG12	1:1513:A:HIS:HB3	6	0.84	0.33	1.0
(1,47)	1:1518:A:VAL:HG12	1:1513:A:HIS:HB2	6	0.84	0.33	1.0
(1,47)	1:1518:A:VAL:HG13	1:1520:A:ASN:HB3	6	0.84	0.33	1.0
(1,89)	1:1511:A:ASN:HB3	1:1521:A:PRO:HG3	6	0.84	0.15	0.84
(1,89)	1:1511:A:ASN:HB2	1:1508:A:MET:HE1	6	0.84	0.15	0.84
(1,89)	1:1511:A:ASN:HB2	1:1521:A:PRO:HG3	6	0.84	0.15	0.84
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	6	0.83	0.13	0.86
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	6	0.73	0.35	0.77
(1,301)	2:38:B:ARG:H	2:33:B:SER:HB3	6	0.73	0.35	0.77
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG21	6	0.66	0.5	0.56
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG22	6	0.66	0.5	0.56
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	6	0.65	0.11	0.7
(1,76)	1:1597:A:PRO:HB3	1:1596:A:SER:HB3	6	0.65	0.11	0.7
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG11	6	0.62	0.74	0.3
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG13	6	0.62	0.74	0.3
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG12	6	0.62	0.74	0.3
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	6	0.57	0.18	0.6
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE2	6	0.52	0.38	0.29
(1,587)	1:1548:A:VAL:HG12	1:1542:A:TYR:HE2	6	0.52	0.38	0.29
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE1	6	0.52	0.38	0.29
(1,2274)	2:14:B:VAL:HG23	2:18:B:GLN:HG3	6	0.52	0.35	0.42
(1,2274)	2:14:B:VAL:HG22	2:18:B:GLN:HG3	6	0.52	0.35	0.42
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	6	0.5	0.02	0.5
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	6	0.49	0.22	0.54
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	6	0.48	0.13	0.51
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	6	0.46	0.01	0.47
(1,1712)	1:1572:A:ILE:HG22	1:1596:A:SER:H	6	0.44	0.17	0.52
(1,1712)	1:1572:A:ILE:HG23	1:1596:A:SER:H	6	0.44	0.17	0.52
(1,1712)	1:1572:A:ILE:HG21	1:1596:A:SER:H	6	0.44	0.17	0.52
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA2	6	0.44	0.17	0.42
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA3	6	0.44	0.17	0.42
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	6	0.37	0.18	0.36
(1,317)	2:53:B:LEU:H	1:1601:A:LYS:HB2	6	0.37	0.21	0.36
(1,317)	2:53:B:LEU:H	2:55:B:LEU:HB3	6	0.37	0.21	0.36
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	6	0.36	0.07	0.38
(1,2567)	2:18:B:GLN:HE22	1:1546:A:GLY:HA3	6	0.36	0.07	0.38
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD22	6	0.34	0.16	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD23	6	0.34	0.16	0.31
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD23	6	0.34	0.04	0.32
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD22	6	0.34	0.04	0.32
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD21	6	0.34	0.04	0.32
(1,470)	1:1572:A:ILE:HG21	1:1596:A:SER:HA	6	0.33	0.07	0.32
(1,470)	1:1572:A:ILE:HG22	1:1596:A:SER:HA	6	0.33	0.07	0.32
(1,470)	1:1572:A:ILE:HG23	1:1596:A:SER:HA	6	0.33	0.07	0.32
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	6	0.31	0.1	0.32
(1,2438)	2:8:B:LEU:HD21	2:8:B:LEU:HA	6	0.31	0.07	0.3
(1,2438)	2:8:B:LEU:HD23	2:8:B:LEU:HA	6	0.31	0.07	0.3
(1,2438)	2:8:B:LEU:HD22	2:8:B:LEU:HA	6	0.31	0.07	0.3
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG2	6	0.3	0.1	0.32
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG3	6	0.3	0.1	0.32
(1,18)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	6	0.3	0.13	0.26
(1,18)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	6	0.3	0.13	0.26
(1,18)	1:1645:A:ALA:HB3	1:1646:A:CYS:HB2	6	0.3	0.13	0.26
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	6	0.28	0.08	0.26
(1,705)	1:1581:A:LEU:HD13	1:1518:A:VAL:H	6	0.27	0.12	0.24
(1,705)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	6	0.27	0.12	0.24
(1,705)	1:1581:A:LEU:HD12	1:1518:A:VAL:H	6	0.27	0.12	0.24
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	6	0.26	0.08	0.28
(1,774)	1:1509:A:LYS:HB3	1:1508:A:MET:HA	6	0.26	0.08	0.28
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	6	0.24	0.14	0.18
(1,512)	1:1645:A:ALA:HB2	1:1614:A:CYS:H	6	0.21	0.09	0.18
(1,512)	1:1645:A:ALA:HB1	1:1614:A:CYS:H	6	0.21	0.09	0.18
(1,512)	1:1645:A:ALA:HB3	1:1614:A:CYS:H	6	0.21	0.09	0.18
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD23	6	0.21	0.12	0.16
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD21	6	0.21	0.12	0.16
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD22	6	0.21	0.12	0.16
(1,195)	1:1604:A:LEU:HD12	1:1633:A:THR:H	6	0.21	0.12	0.16
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	6	0.21	0.08	0.2
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	6	0.2	0.01	0.2
(1,589)	1:1635:A:THR:HG23	1:1637:A:PHE:HA	6	0.2	0.07	0.18
(1,589)	1:1635:A:THR:HG22	1:1637:A:PHE:HA	6	0.2	0.07	0.18
(1,589)	1:1635:A:THR:HG21	1:1637:A:PHE:HA	6	0.2	0.07	0.18
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG13	6	0.14	0.02	0.14
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG11	6	0.14	0.02	0.14
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG12	6	0.14	0.02	0.14
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	6	0.14	0.02	0.13
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD3	6	0.14	0.02	0.14
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	6	0.14	0.02	0.14
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	6	0.12	0.01	0.12
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	6	0.12	0.01	0.12
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	6	0.11	0.01	0.11
(1,2537)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	5	1.9	1.39	2.17
(1,2537)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	5	1.9	1.39	2.17
(1,2301)	2:20:B:VAL:HG13	2:60:B:CYS:HB2	5	1.55	1.01	2.07
(1,2301)	2:20:B:VAL:HG11	2:60:B:CYS:HB2	5	1.55	1.01	2.07
(1,2294)	2:17:B:LEU:HD22	2:16:B:THR:H	5	1.26	0.27	1.18
(1,2294)	2:17:B:LEU:HD23	2:16:B:THR:H	5	1.26	0.27	1.18
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG21	5	1.15	1.23	0.2
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG22	5	1.15	1.23	0.2
(1,275)	2:13:B:LEU:HD22	2:8:B:LEU:HA	5	1.14	1.03	0.89
(1,275)	2:13:B:LEU:HD21	2:8:B:LEU:HA	5	1.14	1.03	0.89
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD22	5	1.1	0.08	1.08
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD23	5	1.1	0.08	1.08
(1,2507)	2:14:B:VAL:HG23	2:17:B:LEU:HD23	5	0.71	0.32	0.81
(1,2507)	2:14:B:VAL:HG22	2:17:B:LEU:HD23	5	0.71	0.32	0.81
(1,2507)	2:14:B:VAL:HG21	2:17:B:LEU:HD22	5	0.71	0.32	0.81
(1,2507)	2:14:B:VAL:HG23	2:17:B:LEU:HD21	5	0.71	0.32	0.81
(1,700)	1:1590:A:LEU:HD22	1:1581:A:LEU:HA	5	0.68	0.91	0.25
(1,700)	1:1590:A:LEU:HD21	1:1581:A:LEU:HA	5	0.68	0.91	0.25
(1,700)	1:1590:A:LEU:HD23	1:1581:A:LEU:HA	5	0.68	0.91	0.25
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	5	0.61	0.15	0.64
(1,22)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	5	0.61	0.35	0.78
(1,22)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	5	0.61	0.35	0.78
(1,22)	1:1584:A:VAL:HG11	1:1583:A:TYR:H	5	0.61	0.35	0.78
(1,22)	1:1584:A:VAL:HG13	1:1583:A:TYR:H	5	0.61	0.35	0.78
(1,26)	1:1591:A:VAL:HG13	1:1593:A:LYS:HE3	5	0.6	0.35	0.46
(1,26)	1:1591:A:VAL:HG13	1:1607:A:LYS:HE3	5	0.6	0.35	0.46
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	5	0.58	0.4	0.41
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	5	0.56	0.31	0.64
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	5	0.52	0.23	0.54
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB3	5	0.51	0.54	0.27
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB2	5	0.51	0.54	0.27
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG12	5	0.47	0.21	0.45
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG11	5	0.47	0.21	0.45
(1,1848)	1:1539:A:THR:HG23	1:1539:A:THR:H	5	0.46	0.04	0.48
(1,1848)	1:1539:A:THR:HG21	1:1539:A:THR:H	5	0.46	0.04	0.48
(1,574)	1:1547:A:VAL:HG11	1:1539:A:THR:HB	5	0.43	0.04	0.42
(1,574)	1:1547:A:VAL:HG12	1:1539:A:THR:HB	5	0.43	0.04	0.42
(1,574)	1:1547:A:VAL:HG13	1:1539:A:THR:HB	5	0.43	0.04	0.42
(1,622)	1:1644:A:LEU:HD13	1:1532:A:LEU:HD22	5	0.43	0.19	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,622)	1:1644:A:LEU:HD11	1:1532:A:LEU:HD22	5	0.43	0.19	0.47
(1,622)	1:1644:A:LEU:HD11	1:1532:A:LEU:HD21	5	0.43	0.19	0.47
(1,622)	1:1644:A:LEU:HD12	1:1532:A:LEU:HD22	5	0.43	0.19	0.47
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE1	5	0.41	0.25	0.36
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE2	5	0.41	0.25	0.36
(1,2459)	2:56:B:LEU:HD22	2:53:B:LEU:HB2	5	0.37	0.17	0.33
(1,2459)	2:56:B:LEU:HD21	2:53:B:LEU:HB2	5	0.37	0.17	0.33
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	5	0.35	0.14	0.39
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	5	0.35	0.2	0.24
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB3	5	0.33	0.11	0.28
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB2	5	0.33	0.11	0.28
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	5	0.33	0.15	0.35
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	5	0.33	0.04	0.31
(1,1494)	1:1510:A:SER:HB3	1:1511:A:ASN:H	5	0.32	0.11	0.37
(1,1494)	1:1510:A:SER:HB2	1:1511:A:ASN:H	5	0.32	0.11	0.37
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE1	5	0.31	0.12	0.29
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE2	5	0.31	0.12	0.29
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD11	5	0.31	0.14	0.33
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD12	5	0.31	0.14	0.33
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD13	5	0.31	0.14	0.33
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG13	5	0.31	0.11	0.31
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG21	5	0.31	0.11	0.31
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG11	5	0.31	0.11	0.31
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG23	5	0.31	0.11	0.31
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	5	0.3	0.06	0.28
(1,368)	1:1542:A:TYR:HE1	2:19:B:PHE:HA	5	0.3	0.15	0.26
(1,368)	1:1542:A:TYR:HE1	1:1543:A:SER:HB2	5	0.3	0.15	0.26
(1,2913)	2:27:B:TYR:HD2	2:27:B:TYR:HA	5	0.29	0.11	0.3
(1,2913)	2:27:B:TYR:HD1	2:27:B:TYR:HA	5	0.29	0.11	0.3
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	5	0.29	0.02	0.29
(1,147)	1:1638:A:PHE:HD2	1:1610:A:ILE:HD13	5	0.28	0.28	0.14
(1,147)	1:1638:A:PHE:HD1	1:1610:A:ILE:HD13	5	0.28	0.28	0.14
(1,147)	1:1638:A:PHE:HD2	1:1610:A:ILE:HD11	5	0.28	0.28	0.14
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	5	0.28	0.14	0.31
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB3	5	0.27	0.22	0.19
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB2	5	0.27	0.22	0.19
(1,2286)	2:42:B:ILE:HD11	2:28:B:PHE:HD2	5	0.27	0.06	0.31
(1,2286)	2:42:B:ILE:HD13	2:28:B:PHE:HD1	5	0.27	0.06	0.31
(1,2286)	2:42:B:ILE:HD12	2:28:B:PHE:HD2	5	0.27	0.06	0.31
(1,2286)	2:42:B:ILE:HD12	2:28:B:PHE:HD1	5	0.27	0.06	0.31
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	5	0.25	0.05	0.26
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	5	0.24	0.08	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,21)	1:1645:A:ALA:HB1	1:1612:A:PHE:HA	5	0.23	0.08	0.21
(1,21)	1:1645:A:ALA:HB3	1:1612:A:PHE:HA	5	0.23	0.08	0.21
(1,21)	1:1645:A:ALA:HB2	1:1612:A:PHE:HA	5	0.23	0.08	0.21
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	5	0.23	0.1	0.19
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	5	0.23	0.05	0.24
(1,596)	1:1529:A:LEU:HD23	1:1645:A:ALA:HA	5	0.22	0.07	0.27
(1,596)	1:1529:A:LEU:HD21	1:1645:A:ALA:HA	5	0.22	0.07	0.27
(1,596)	1:1529:A:LEU:HD22	1:1645:A:ALA:HA	5	0.22	0.07	0.27
(1,465)	1:1625:A:MET:HE3	1:1625:A:MET:H	5	0.22	0.03	0.2
(1,465)	1:1625:A:MET:HE2	1:1625:A:MET:H	5	0.22	0.03	0.2
(1,542)	1:1613:A:VAL:HG13	1:1641:A:HIS:HA	5	0.21	0.09	0.22
(1,542)	1:1613:A:VAL:HG11	1:1641:A:HIS:HA	5	0.21	0.09	0.22
(1,542)	1:1613:A:VAL:HG12	1:1641:A:HIS:HA	5	0.21	0.09	0.22
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	5	0.2	0.06	0.19
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	5	0.19	0.06	0.18
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	5	0.19	0.07	0.18
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD12	5	0.19	0.09	0.15
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD11	5	0.19	0.09	0.15
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD13	5	0.19	0.09	0.15
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	5	0.18	0.03	0.18
(1,149)	1:1638:A:PHE:HD1	1:1540:A:ALA:HB1	5	0.18	0.05	0.17
(1,149)	1:1638:A:PHE:HD2	1:1636:A:LEU:HD21	5	0.18	0.05	0.17
(1,149)	1:1638:A:PHE:HD2	1:1540:A:ALA:HB3	5	0.18	0.05	0.17
(1,149)	1:1638:A:PHE:HD1	1:1540:A:ALA:HB2	5	0.18	0.05	0.17
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	5	0.17	0.04	0.15
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	5	0.17	0.07	0.14
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	5	0.17	0.02	0.16
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG21	5	0.17	0.04	0.16
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG22	5	0.17	0.04	0.16
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG22	5	0.17	0.05	0.14
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG23	5	0.17	0.05	0.14
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG21	5	0.17	0.05	0.14
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	5	0.16	0.05	0.18
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	5	0.16	0.03	0.17
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	5	0.14	0.01	0.14
(1,6)	1:1552:A:ILE:HD11	1:1610:A:ILE:HB	5	0.14	0.02	0.14
(1,6)	1:1552:A:ILE:HD13	1:1610:A:ILE:HB	5	0.14	0.02	0.14
(1,6)	1:1552:A:ILE:HD11	1:1532:A:LEU:HB2	5	0.14	0.02	0.14
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	5	0.13	0.03	0.12
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	5	0.13	0.03	0.12
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	5	0.12	0.01	0.12
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	5	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,55)	1:1518:A:VAL:HG13	1:1511:A:ASN:HB2	4	1.21	0.74	1.22
(1,55)	1:1518:A:VAL:HG13	1:1511:A:ASN:HB3	4	1.21	0.74	1.22
(1,55)	1:1518:A:VAL:HG12	1:1511:A:ASN:HB2	4	1.21	0.74	1.22
(1,2186)	1:1556:A:ASN:HD22	1:1537:A:GLY:HA2	4	0.89	0.56	0.92
(1,650)	1:1590:A:LEU:HD21	1:1581:A:LEU:H	4	0.85	1.13	0.25
(1,650)	1:1590:A:LEU:HD23	1:1581:A:LEU:H	4	0.85	1.13	0.25
(1,650)	1:1590:A:LEU:HD22	1:1581:A:LEU:H	4	0.85	1.13	0.25
(1,1858)	1:1602:A:SER:HB2	1:1602:A:SER:H	4	0.8	0.04	0.82
(1,388)	2:23:B:ASP:HB3	2:22:B:GLY:H	4	0.78	0.08	0.8
(1,388)	2:16:B:THR:H	2:12:B:GLU:HG3	4	0.78	0.08	0.8
(1,1396)	1:1591:A:VAL:HG13	1:1591:A:VAL:H	4	0.76	0.04	0.74
(1,1396)	1:1591:A:VAL:HG12	1:1591:A:VAL:H	4	0.76	0.04	0.74
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD23	4	0.67	0.54	0.48
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD21	4	0.67	0.54	0.48
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD22	4	0.67	0.54	0.48
(1,1063)	1:1644:A:LEU:HD11	1:1644:A:LEU:HB3	4	0.64	0.07	0.64
(1,1063)	1:1644:A:LEU:HD13	1:1644:A:LEU:HB3	4	0.64	0.07	0.64
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG22	4	0.62	0.06	0.64
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG21	4	0.62	0.06	0.64
(1,387)	1:1572:A:ILE:HD11	2:16:B:THR:H	4	0.57	0.21	0.56
(1,387)	1:1572:A:ILE:HD12	2:16:B:THR:H	4	0.57	0.21	0.56
(1,387)	1:1572:A:ILE:HD13	2:16:B:THR:H	4	0.57	0.21	0.56
(1,795)	1:1617:A:GLU:HG3	1:1617:A:GLU:H	4	0.54	0.03	0.54
(1,795)	1:1617:A:GLU:HG2	1:1617:A:GLU:H	4	0.54	0.03	0.54
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB1	4	0.53	0.46	0.37
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB2	4	0.53	0.46	0.37
(1,2992)	2:42:B:ILE:HD11	2:59:B:TYR:HE2	4	0.5	0.25	0.56
(1,2992)	2:42:B:ILE:HD13	2:59:B:TYR:HE2	4	0.5	0.25	0.56
(1,2992)	2:42:B:ILE:HD12	2:59:B:TYR:HE2	4	0.5	0.25	0.56
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD21	4	0.46	0.2	0.5
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD23	4	0.46	0.2	0.5
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD22	4	0.46	0.2	0.5
(1,497)	1:1645:A:ALA:HB2	1:1529:A:LEU:HD12	4	0.46	0.24	0.37
(1,497)	1:1645:A:ALA:HB1	1:1529:A:LEU:HD12	4	0.46	0.24	0.37
(1,497)	1:1645:A:ALA:HB3	1:1529:A:LEU:HD11	4	0.46	0.24	0.37
(1,918)	1:1570:A:THR:HG21	1:1570:A:THR:HA	4	0.44	0.02	0.44
(1,2382)	2:55:B:LEU:HD23	2:51:B:CYS:HA	4	0.43	0.17	0.5
(1,2382)	2:55:B:LEU:HD21	2:51:B:CYS:HA	4	0.43	0.17	0.5
(1,15)	1:1577:A:ALA:HB1	1:1555:A:GLU:HG2	4	0.43	0.22	0.44
(1,15)	1:1577:A:ALA:HB3	1:1555:A:GLU:HG2	4	0.43	0.22	0.44
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE1	4	0.42	0.23	0.32
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE2	4	0.42	0.23	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,185)	1:1632:A:GLN:H	2:53:B:LEU:HD21	4	0.42	0.18	0.47
(1,185)	1:1632:A:GLN:H	1:1629:A:LEU:HD13	4	0.42	0.18	0.47
(1,185)	1:1632:A:GLN:H	2:53:B:LEU:HD22	4	0.42	0.18	0.47
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG22	4	0.38	0.18	0.4
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG23	4	0.38	0.18	0.4
(1,2105)	1:1612:A:PHE:H	1:1611:A:SER:HB2	4	0.38	0.1	0.41
(1,2501)	2:56:B:LEU:HD13	2:20:B:VAL:HG13	4	0.38	0.14	0.4
(1,2501)	2:56:B:LEU:HD11	2:20:B:VAL:HG13	4	0.38	0.14	0.4
(1,2501)	2:56:B:LEU:HD11	2:20:B:VAL:HG11	4	0.38	0.14	0.4
(1,2501)	2:56:B:LEU:HD13	2:20:B:VAL:HG11	4	0.38	0.14	0.4
(1,3019)	2:18:B:GLN:HG3	1:1545:A:SER:HB3	4	0.37	0.18	0.32
(1,116)	1:1613:A:VAL:HG13	1:1642:A:THR:H	4	0.33	0.25	0.22
(1,116)	1:1613:A:VAL:HG11	1:1642:A:THR:H	4	0.33	0.25	0.22
(1,181)	1:1616:A:PRO:HB3	1:1617:A:GLU:H	4	0.32	0.04	0.34
(1,181)	1:1617:A:GLU:H	1:1617:A:GLU:HG3	4	0.32	0.04	0.34
(1,370)	2:18:B:GLN:HG2	1:1569:A:GLN:HE21	4	0.32	0.21	0.26
(1,370)	2:18:B:GLN:HG2	1:1542:A:TYR:HD1	4	0.32	0.21	0.26
(1,597)	1:1529:A:LEU:HD21	1:1529:A:LEU:HA	4	0.32	0.26	0.18
(1,597)	1:1529:A:LEU:HD22	1:1529:A:LEU:HA	4	0.32	0.26	0.18
(1,597)	1:1529:A:LEU:HD23	1:1529:A:LEU:HA	4	0.32	0.26	0.18
(1,2246)	1:1583:A:TYR:HE1	1:1522:A:SER:H	4	0.3	0.07	0.3
(1,2246)	1:1583:A:TYR:HE2	1:1522:A:SER:H	4	0.3	0.07	0.3
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB1	4	0.29	0.23	0.18
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB3	4	0.29	0.23	0.18
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB2	4	0.29	0.23	0.18
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD1	4	0.28	0.13	0.29
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD2	4	0.28	0.13	0.29
(1,832)	1:1581:A:LEU:HD23	1:1590:A:LEU:HB2	4	0.28	0.13	0.26
(1,832)	1:1581:A:LEU:HD21	1:1590:A:LEU:HB2	4	0.28	0.13	0.26
(1,310)	2:43:B:VAL:H	2:45:B:GLU:HB2	4	0.28	0.21	0.19
(1,169)	1:1512:A:GLU:H	1:1518:A:VAL:HG12	4	0.27	0.03	0.27
(1,169)	1:1520:A:ASN:H	1:1518:A:VAL:HG12	4	0.27	0.03	0.27
(1,169)	1:1512:A:GLU:H	1:1518:A:VAL:HG11	4	0.27	0.03	0.27
(1,53)	1:1588:A:LEU:HD12	1:1583:A:TYR:H	4	0.27	0.11	0.25
(1,53)	1:1588:A:LEU:HD11	1:1583:A:TYR:H	4	0.27	0.11	0.25
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG21	4	0.26	0.1	0.22
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG23	4	0.26	0.1	0.22
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG22	4	0.26	0.1	0.22
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG22	4	0.26	0.01	0.26
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG23	4	0.26	0.01	0.26
(1,67)	1:1601:A:LYS:HG3	1:1600:A:SER:HB2	4	0.26	0.05	0.26
(1,67)	1:1601:A:LYS:HG2	1:1600:A:SER:HB2	4	0.26	0.05	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,444)	1:1550:A:MET:HE1	1:1610:A:ILE:HA	4	0.26	0.11	0.22
(1,444)	1:1550:A:MET:HE2	1:1610:A:ILE:HA	4	0.26	0.11	0.22
(1,958)	1:1627:A:ILE:HD12	1:1641:A:HIS:HD2	4	0.25	0.04	0.24
(1,958)	1:1627:A:ILE:HD11	1:1641:A:HIS:HD2	4	0.25	0.04	0.24
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB3	4	0.24	0.05	0.24
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB1	4	0.24	0.05	0.24
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB2	4	0.24	0.05	0.24
(1,2471)	2:38:B:ARG:H	2:37:B:ARG:HG2	4	0.22	0.05	0.23
(1,2471)	2:37:B:ARG:HG3	2:38:B:ARG:H	4	0.22	0.05	0.23
(1,2480)	2:13:B:LEU:HD11	2:13:B:LEU:HA	4	0.22	0.08	0.23
(1,2480)	2:13:B:LEU:HD13	2:13:B:LEU:HA	4	0.22	0.08	0.23
(1,2480)	2:13:B:LEU:HD12	2:13:B:LEU:HA	4	0.22	0.08	0.23
(1,1072)	1:1590:A:LEU:HD22	1:1553:A:CYS:HA	4	0.2	0.08	0.18
(1,1072)	1:1590:A:LEU:HD21	1:1553:A:CYS:HA	4	0.2	0.08	0.18
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD21	4	0.18	0.06	0.16
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD23	4	0.18	0.06	0.16
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD22	4	0.18	0.06	0.16
(1,1287)	1:1635:A:THR:HG21	1:1609:A:VAL:H	4	0.18	0.05	0.19
(1,1287)	1:1635:A:THR:HG22	1:1609:A:VAL:H	4	0.18	0.05	0.19
(1,46)	1:1540:A:ALA:HB2	1:1541:A:ALA:HA	4	0.18	0.04	0.18
(1,46)	1:1540:A:ALA:HB3	1:1541:A:ALA:HA	4	0.18	0.04	0.18
(1,46)	1:1540:A:ALA:HB1	1:1541:A:ALA:HA	4	0.18	0.04	0.18
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG3	4	0.17	0.04	0.18
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG2	4	0.17	0.04	0.18
(1,2524)	2:64:B:ALA:HA	2:65:B:LYS:HB2	4	0.17	0.04	0.18
(1,823)	1:1623:A:ARG:HD2	1:1623:A:ARG:HE	4	0.17	0.04	0.16
(1,1395)	1:1591:A:VAL:H	1:1590:A:LEU:HB3	4	0.16	0.02	0.16
(1,1029)	1:1610:A:ILE:HG22	1:1640:A:TRP:HZ3	4	0.16	0.03	0.16
(1,1029)	1:1610:A:ILE:HG23	1:1640:A:TRP:HZ3	4	0.16	0.03	0.16
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG23	4	0.16	0.03	0.15
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG21	4	0.16	0.03	0.15
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE1	4	0.15	0.04	0.14
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE2	4	0.15	0.04	0.14
(1,2962)	2:18:B:GLN:HG2	2:26:B:PHE:HE2	4	0.14	0.01	0.14
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG23	4	0.13	0.02	0.14
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG22	4	0.13	0.02	0.14
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG21	4	0.13	0.02	0.14
(1,2236)	1:1549:A:TYR:HD1	1:1556:A:ASN:HD21	4	0.12	0.03	0.1
(1,2632)	2:38:B:ARG:H	2:38:B:ARG:HB3	4	0.12	0.01	0.12
(1,1651)	1:1617:A:GLU:H	1:1615:A:ARG:HA	4	0.12	0.02	0.12
(1,1988)	1:1520:A:ASN:H	1:1523:A:THR:H	4	0.11	0.0	0.11
(1,1944)	1:1633:A:THR:HG22	1:1633:A:THR:H	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1944)	1:1633:A:THR:HG23	1:1633:A:THR:H	4	0.11	0.0	0.11
(1,1944)	1:1633:A:THR:HG21	1:1633:A:THR:H	4	0.11	0.0	0.11
(1,1449)	1:1589:A:GLN:H	1:1584:A:VAL:HG21	3	3.13	0.17	3.04
(1,1449)	1:1589:A:GLN:H	1:1584:A:VAL:HG23	3	3.13	0.17	3.04
(1,2276)	2:14:B:VAL:HG21	2:28:B:PHE:HE2	3	2.12	0.13	2.16
(1,2276)	2:14:B:VAL:HG23	2:28:B:PHE:HE1	3	2.12	0.13	2.16
(1,2276)	2:14:B:VAL:HG22	2:28:B:PHE:HE1	3	2.12	0.13	2.16
(1,2450)	2:55:B:LEU:HD13	2:58:B:THR:HG21	3	2.01	1.43	1.02
(1,2450)	2:55:B:LEU:HD11	2:58:B:THR:HG23	3	2.01	1.43	1.02
(1,2450)	2:55:B:LEU:HD12	2:58:B:THR:HG23	3	2.01	1.43	1.02
(1,1202)	1:1584:A:VAL:H	1:1584:A:VAL:HG23	3	1.68	0.08	1.64
(1,1202)	1:1584:A:VAL:H	1:1584:A:VAL:HG22	3	1.68	0.08	1.64
(1,2961)	2:56:B:LEU:HD23	2:53:B:LEU:H	3	1.68	1.23	1.64
(1,2527)	2:58:B:THR:HG22	2:59:B:TYR:HB3	3	1.62	0.42	1.88
(1,2527)	2:58:B:THR:HG21	2:59:B:TYR:HB3	3	1.62	0.42	1.88
(1,2527)	2:58:B:THR:HG23	2:59:B:TYR:HB3	3	1.62	0.42	1.88
(1,237)	2:20:B:VAL:HG23	2:26:B:PHE:HD2	3	1.61	0.26	1.72
(1,237)	2:20:B:VAL:HG22	2:26:B:PHE:HD2	3	1.61	0.26	1.72
(1,971)	1:1608:A:SER:HA	1:1636:A:LEU:HD23	3	1.38	0.15	1.45
(1,971)	1:1608:A:SER:HA	1:1636:A:LEU:HD22	3	1.38	0.15	1.45
(1,2302)	2:20:B:VAL:HG11	2:17:B:LEU:HA	3	1.3	0.09	1.24
(1,694)	1:1636:A:LEU:HD13	1:1635:A:THR:HA	3	1.26	0.36	1.12
(1,694)	1:1636:A:LEU:HD11	1:1635:A:THR:HA	3	1.26	0.36	1.12
(1,889)	1:1544:A:LYS:HA	1:1544:A:LYS:HD2	3	1.12	0.08	1.17
(1,1024)	1:1552:A:ILE:HD13	1:1590:A:LEU:HD11	3	1.0	1.0	0.29
(1,1024)	1:1552:A:ILE:HD11	1:1590:A:LEU:HD11	3	1.0	1.0	0.29
(1,1024)	1:1552:A:ILE:HD12	1:1590:A:LEU:HD11	3	1.0	1.0	0.29
(1,535)	1:1584:A:VAL:HG13	1:1584:A:VAL:HA	3	0.93	0.03	0.92
(1,535)	1:1584:A:VAL:HG12	1:1584:A:VAL:HA	3	0.93	0.03	0.92
(1,1587)	1:1604:A:LEU:H	1:1604:A:LEU:HB2	3	0.89	0.06	0.88
(1,1075)	1:1581:A:LEU:HD22	1:1590:A:LEU:HD11	3	0.88	0.99	0.18
(1,1075)	1:1581:A:LEU:HD23	1:1590:A:LEU:HD12	3	0.88	0.99	0.18
(1,2293)	2:17:B:LEU:HD13	2:56:B:LEU:HD11	3	0.8	0.54	0.44
(1,2293)	2:17:B:LEU:HD11	2:56:B:LEU:HD11	3	0.8	0.54	0.44
(1,367)	1:1593:A:LYS:HE2	1:1580:A:ARG:HE	3	0.77	0.31	0.96
(1,367)	1:1601:A:LYS:HE3	1:1604:A:LEU:H	3	0.77	0.31	0.96
(1,2670)	2:21:B:CYS:H	2:20:B:VAL:HG11	3	0.76	0.01	0.75
(1,187)	1:1567:A:PHE:H	1:1548:A:VAL:HG22	3	0.68	0.74	0.16
(1,187)	1:1567:A:PHE:H	1:1565:A:ALA:HB3	3	0.68	0.74	0.16
(1,187)	1:1567:A:PHE:H	1:1548:A:VAL:HG23	3	0.68	0.74	0.16
(1,2283)	2:42:B:ILE:HD12	2:43:B:VAL:H	3	0.66	0.27	0.85
(1,683)	1:1532:A:LEU:HD12	1:1644:A:LEU:HD13	3	0.65	0.26	0.77

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,683)	1:1532:A:LEU:HD13	1:1644:A:LEU:HD11	3	0.65	0.26	0.77
(1,683)	1:1532:A:LEU:HD11	1:1644:A:LEU:HD13	3	0.65	0.26	0.77
(1,1450)	1:1589:A:GLN:H	1:1581:A:LEU:HD12	3	0.64	0.7	0.15
(1,1450)	1:1589:A:GLN:H	1:1581:A:LEU:HD11	3	0.64	0.7	0.15
(1,402)	1:1629:A:LEU:HB3	2:19:B:PHE:HE2	3	0.63	0.29	0.75
(1,234)	2:55:B:LEU:HD13	2:58:B:THR:HG21	3	0.63	0.09	0.59
(1,234)	2:55:B:LEU:HD11	2:58:B:THR:HG23	3	0.63	0.09	0.59
(1,234)	2:55:B:LEU:HD12	2:54:B:ALA:HB3	3	0.63	0.09	0.59
(1,660)	1:1636:A:LEU:HD12	1:1636:A:LEU:HA	3	0.62	0.09	0.64
(1,660)	1:1636:A:LEU:HD13	1:1636:A:LEU:HA	3	0.62	0.09	0.64
(1,3011)	2:13:B:LEU:HB3	2:13:B:LEU:H	3	0.62	0.31	0.78
(1,1054)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	3	0.56	0.3	0.65
(1,2418)	2:63:B:PRO:HD3	2:63:B:PRO:HB3	3	0.56	0.02	0.55
(1,2984)	2:20:B:VAL:HA	2:20:B:VAL:HG23	3	0.56	0.0	0.56
(1,2984)	2:20:B:VAL:HA	2:20:B:VAL:HG22	3	0.56	0.0	0.56
(1,733)	1:1582:A:ARG:HG2	1:1582:A:ARG:H	3	0.55	0.1	0.49
(1,2339)	2:18:B:GLN:HG3	2:26:B:PHE:HD1	3	0.54	0.28	0.58
(1,2339)	2:18:B:GLN:HG3	2:26:B:PHE:HD2	3	0.54	0.28	0.58
(1,2619)	2:37:B:ARG:H	2:37:B:ARG:HG3	3	0.54	0.08	0.55
(1,2619)	2:37:B:ARG:H	2:37:B:ARG:HG2	3	0.54	0.08	0.55
(1,904)	1:1601:A:LYS:HG2	1:1602:A:SER:HB2	3	0.53	0.21	0.52
(1,904)	1:1601:A:LYS:HG2	1:1602:A:SER:HB3	3	0.53	0.21	0.52
(1,904)	1:1601:A:LYS:HG3	1:1602:A:SER:HB3	3	0.53	0.21	0.52
(1,609)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	3	0.52	0.3	0.61
(1,711)	1:1604:A:LEU:HD22	1:1605:A:SER:H	3	0.5	0.09	0.54
(1,711)	1:1604:A:LEU:HD23	1:1605:A:SER:H	3	0.5	0.09	0.54
(1,2975)	2:17:B:LEU:HD11	2:17:B:LEU:HB3	3	0.5	0.02	0.5
(1,2975)	2:17:B:LEU:HD12	2:17:B:LEU:HB3	3	0.5	0.02	0.5
(1,399)	2:19:B:PHE:HD2	2:16:B:THR:HG22	3	0.49	0.23	0.47
(1,399)	2:19:B:PHE:HD2	2:16:B:THR:HG23	3	0.49	0.23	0.47
(1,714)	1:1604:A:LEU:HD22	1:1604:A:LEU:HA	3	0.49	0.02	0.48
(1,714)	1:1604:A:LEU:HD12	1:1604:A:LEU:HA	3	0.49	0.02	0.48
(1,714)	1:1604:A:LEU:HD11	1:1604:A:LEU:HA	3	0.49	0.02	0.48
(1,2440)	2:17:B:LEU:HD22	2:17:B:LEU:HA	3	0.48	0.07	0.46
(1,2440)	2:17:B:LEU:HD21	2:17:B:LEU:HA	3	0.48	0.07	0.46
(1,84)	1:1512:A:GLU:HG2	1:1582:A:ARG:HD2	3	0.47	0.33	0.37
(1,84)	1:1589:A:GLN:HG2	1:1582:A:ARG:HD3	3	0.47	0.33	0.37
(1,84)	1:1589:A:GLN:HG2	1:1582:A:ARG:HD2	3	0.47	0.33	0.37
(1,2817)	2:20:B:VAL:H	2:19:B:PHE:HE2	3	0.46	0.11	0.43
(1,369)	2:16:B:THR:H	1:1570:A:THR:HG22	3	0.46	0.27	0.28
(1,369)	2:16:B:THR:H	1:1570:A:THR:HG21	3	0.46	0.27	0.28
(1,676)	1:1529:A:LEU:HD13	1:1529:A:LEU:HB3	3	0.45	0.49	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2305)	2:20:B:VAL:HG11	2:17:B:LEU:HA	3	0.38	0.09	0.32
(1,1620)	1:1558:A:ASN:H	1:1557:A:GLU:HG2	3	0.37	0.35	0.13
(1,3013)	1:1629:A:LEU:HD12	2:19:B:PHE:HZ	3	0.37	0.17	0.34
(1,193)	1:1575:A:GLY:H	1:1606:A:TYR:HB3	3	0.35	0.07	0.31
(1,1895)	1:1545:A:SER:H	1:1543:A:SER:HB2	3	0.35	0.06	0.39
(1,2542)	2:50:B:SER:H	2:50:B:SER:HB3	3	0.35	0.06	0.31
(1,664)	1:1607:A:LYS:HG3	1:1607:A:LYS:HE3	3	0.34	0.18	0.35
(1,493)	1:1577:A:ALA:HB3	1:1565:A:ALA:H	3	0.33	0.07	0.36
(1,493)	1:1577:A:ALA:HB2	1:1565:A:ALA:H	3	0.33	0.07	0.36
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG11	3	0.33	0.19	0.26
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG13	3	0.33	0.19	0.26
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG12	3	0.33	0.19	0.26
(1,363)	1:1632:A:GLN:H	2:53:B:LEU:HD21	3	0.31	0.06	0.28
(1,363)	1:1632:A:GLN:H	1:1629:A:LEU:HD13	3	0.31	0.06	0.28
(1,363)	1:1632:A:GLN:H	2:53:B:LEU:HD22	3	0.31	0.06	0.28
(1,1420)	1:1588:A:LEU:H	1:1612:A:PHE:HB2	3	0.3	0.1	0.24
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD21	3	0.28	0.17	0.2
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD22	3	0.28	0.17	0.2
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD23	3	0.28	0.17	0.2
(1,171)	1:1511:A:ASN:HB2	1:1511:A:ASN:H	3	0.27	0.03	0.26
(1,295)	2:35:B:VAL:H	2:34:B:ARG:HG2	3	0.27	0.16	0.19
(1,782)	1:1569:A:GLN:HG2	1:1570:A:THR:H	3	0.27	0.11	0.27
(1,2922)	2:61:B:ALA:HA	2:27:B:TYR:HD2	3	0.27	0.18	0.16
(1,2922)	2:61:B:ALA:HA	2:27:B:TYR:HD1	3	0.27	0.18	0.16
(1,1092)	1:1581:A:LEU:HD13	1:1518:A:VAL:H	3	0.26	0.06	0.29
(1,1092)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	3	0.26	0.06	0.29
(1,2519)	2:63:B:PRO:HB3	2:62:B:THR:HA	3	0.26	0.05	0.27
(1,2386)	2:33:B:SER:H	2:33:B:SER:HB3	3	0.25	0.02	0.26
(1,293)	2:54:B:ALA:H	2:56:B:LEU:HD23	3	0.25	0.13	0.2
(1,293)	2:54:B:ALA:H	2:53:B:LEU:HD23	3	0.25	0.13	0.2
(1,293)	2:54:B:ALA:H	2:53:B:LEU:HD22	3	0.25	0.13	0.2
(1,2699)	2:3:B:ARG:H	2:3:B:ARG:HB3	3	0.25	0.1	0.22
(1,974)	1:1533:A:SER:HB3	1:1552:A:ILE:HB	3	0.24	0.06	0.28
(1,1076)	1:1526:A:LEU:HD11	1:1528:A:ASP:HB3	3	0.24	0.08	0.25
(1,1076)	1:1526:A:LEU:HD12	1:1528:A:ASP:HB3	3	0.24	0.08	0.25
(1,987)	1:1627:A:ILE:HD13	1:1638:A:PHE:HA	3	0.23	0.05	0.23
(1,987)	1:1627:A:ILE:HD11	1:1638:A:PHE:HA	3	0.23	0.05	0.23
(1,1534)	1:1572:A:ILE:HG21	1:1573:A:SER:H	3	0.22	0.09	0.25
(1,1534)	1:1572:A:ILE:HG22	1:1573:A:SER:H	3	0.22	0.09	0.25
(1,1064)	1:1529:A:LEU:HD12	1:1588:A:LEU:HB3	3	0.21	0.07	0.24
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG11	3	0.21	0.08	0.21
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG12	3	0.21	0.08	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG13	3	0.21	0.08	0.21
(1,1301)	1:1557:A:GLU:H	1:1558:A:ASN:HD22	3	0.21	0.03	0.22
(1,2245)	1:1592:A:TYR:HH	1:1590:A:LEU:HD22	3	0.21	0.07	0.18
(1,2245)	1:1592:A:TYR:HH	1:1590:A:LEU:HD21	3	0.21	0.07	0.18
(1,339)	2:5:B:SER:H	2:5:B:SER:HB2	3	0.2	0.03	0.19
(1,1457)	1:1514:A:ASP:HB2	1:1514:A:ASP:H	3	0.2	0.02	0.21
(1,2330)	2:61:B:ALA:HB3	2:60:B:CYS:HA	3	0.19	0.03	0.18
(1,2330)	2:61:B:ALA:HB1	2:60:B:CYS:HA	3	0.19	0.03	0.18
(1,2330)	2:61:B:ALA:HB2	2:60:B:CYS:HA	3	0.19	0.03	0.18
(1,1965)	1:1568:A:GLY:H	1:1549:A:TYR:HE2	3	0.19	0.04	0.18
(1,1694)	1:1645:A:ALA:H	1:1644:A:LEU:HB3	3	0.18	0.05	0.15
(1,304)	2:9:B:CYS:H	2:13:B:LEU:HD23	3	0.18	0.05	0.16
(1,304)	2:54:B:ALA:H	2:53:B:LEU:HD21	3	0.18	0.05	0.16
(1,787)	1:1617:A:GLU:HG2	1:1617:A:GLU:HA	3	0.18	0.03	0.19
(1,1061)	1:1563:A:VAL:HG13	1:1566:A:CYS:HB3	3	0.18	0.07	0.14
(1,1061)	1:1563:A:VAL:HG12	1:1566:A:CYS:HB3	3	0.18	0.07	0.14
(1,2430)	2:63:B:PRO:HD2	2:63:B:PRO:HB3	3	0.16	0.02	0.15
(1,2531)	2:61:B:ALA:HB3	2:62:B:THR:HA	3	0.16	0.04	0.16
(1,2531)	2:61:B:ALA:HB1	2:62:B:THR:HA	3	0.16	0.04	0.16
(1,1421)	1:1588:A:LEU:H	1:1645:A:ALA:HB1	3	0.15	0.03	0.13
(1,1421)	1:1588:A:LEU:H	1:1645:A:ALA:HB2	3	0.15	0.03	0.13
(1,706)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	3	0.14	0.04	0.14
(1,706)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	3	0.14	0.04	0.14
(1,1085)	1:1636:A:LEU:HD12	1:1574:A:VAL:HG22	3	0.14	0.02	0.15
(1,1085)	1:1636:A:LEU:HD12	1:1574:A:VAL:HG21	3	0.14	0.02	0.15
(1,2604)	2:34:B:ARG:H	2:33:B:SER:HB2	3	0.14	0.03	0.15
(1,834)	1:1590:A:LEU:HB2	1:1590:A:LEU:HA	3	0.13	0.01	0.12
(1,1576)	1:1644:A:LEU:HD23	1:1644:A:LEU:H	3	0.12	0.01	0.12
(1,2078)	1:1582:A:ARG:HA	1:1583:A:TYR:H	3	0.12	0.01	0.12
(1,921)	1:1586:A:GLN:HA	1:1586:A:GLN:HB2	3	0.12	0.0	0.12
(1,2318)	2:33:B:SER:H	2:32:B:ALA:HA	3	0.12	0.02	0.11
(1,2852)	2:23:B:ASP:H	2:22:B:GLY:H	3	0.12	0.0	0.12
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD2	3	0.11	0.02	0.1
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD3	3	0.11	0.02	0.1
(1,1250)	1:1529:A:LEU:HD11	1:1529:A:LEU:H	3	0.11	0.01	0.1
(1,1250)	1:1529:A:LEU:HD13	1:1529:A:LEU:H	3	0.11	0.01	0.1
(1,1159)	1:1592:A:TYR:H	1:1593:A:LYS:H	3	0.1	0.0	0.1
(1,2502)	2:56:B:LEU:HD23	2:53:B:LEU:H	2	2.15	0.79	2.15
(1,1084)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD21	2	2.04	0.05	2.04
(1,1084)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	2	2.04	0.05	2.04
(1,666)	1:1626:A:LEU:HD21	1:1636:A:LEU:HD23	2	1.8	0.05	1.8
(1,666)	1:1626:A:LEU:HD22	1:1636:A:LEU:HD23	2	1.8	0.05	1.8

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,544)	1:1518:A:VAL:HG23	1:1517:A:GLN:HA	2	1.7	0.17	1.7
(1,174)	1:1511:A:ASN:H	1:1518:A:VAL:HG11	2	1.64	0.21	1.64
(1,174)	1:1513:A:HIS:H	1:1518:A:VAL:HG11	2	1.64	0.21	1.64
(1,1747)	1:1567:A:PHE:H	1:1574:A:VAL:HG11	2	1.62	0.02	1.62
(1,1747)	1:1567:A:PHE:H	1:1574:A:VAL:HG12	2	1.62	0.02	1.62
(1,115)	1:1574:A:VAL:HG21	1:1566:A:CYS:H	2	1.57	0.1	1.57
(1,695)	1:1529:A:LEU:HD11	1:1644:A:LEU:HD21	2	1.48	0.07	1.48
(1,695)	1:1529:A:LEU:HD12	1:1644:A:LEU:HD22	2	1.48	0.07	1.48
(1,1053)	1:1574:A:VAL:HG21	1:1565:A:ALA:HB2	2	1.46	0.03	1.46
(1,1053)	1:1574:A:VAL:HG21	1:1565:A:ALA:HB3	2	1.46	0.03	1.46
(1,1058)	1:1626:A:LEU:HD21	1:1638:A:PHE:HD1	2	1.3	1.17	1.3
(1,1058)	1:1626:A:LEU:HD23	1:1638:A:PHE:HD1	2	1.3	1.17	1.3
(1,1591)	1:1518:A:VAL:H	1:1518:A:VAL:HG21	2	1.3	0.01	1.3
(1,2298)	2:55:B:LEU:HD13	2:59:B:TYR:HB2	2	1.3	0.82	1.3
(1,2298)	2:55:B:LEU:HD11	2:56:B:LEU:HA	2	1.3	0.82	1.3
(1,3007)	2:17:B:LEU:H	2:56:B:LEU:HD11	2	1.2	0.08	1.2
(1,3007)	2:17:B:LEU:H	2:56:B:LEU:HD13	2	1.2	0.08	1.2
(1,85)	1:1584:A:VAL:HG21	1:1589:A:GLN:HB3	2	1.15	0.02	1.15
(1,85)	1:1584:A:VAL:HG23	1:1589:A:GLN:HB3	2	1.15	0.02	1.15
(1,1477)	1:1644:A:LEU:HD23	1:1528:A:ASP:H	2	1.12	0.03	1.12
(1,1477)	1:1644:A:LEU:HD21	1:1528:A:ASP:H	2	1.12	0.03	1.12
(1,2868)	2:17:B:LEU:HD11	2:28:B:PHE:HD1	2	1.08	0.29	1.08
(1,2868)	2:17:B:LEU:HD12	2:28:B:PHE:HD1	2	1.08	0.29	1.08
(1,2714)	2:52:B:ASP:H	2:51:B:CYS:HB3	2	0.86	0.13	0.86
(1,642)	1:1518:A:VAL:HG11	1:1518:A:VAL:HA	2	0.86	0.01	0.86
(1,642)	1:1518:A:VAL:HG12	1:1518:A:VAL:HA	2	0.86	0.01	0.86
(1,2437)	2:56:B:LEU:HD11	2:17:B:LEU:HA	2	0.82	0.5	0.82
(1,2437)	2:56:B:LEU:HD13	2:17:B:LEU:HA	2	0.82	0.5	0.82
(1,3015)	1:1636:A:LEU:HD22	2:19:B:PHE:HE2	2	0.82	0.64	0.82
(1,3015)	2:19:B:PHE:HE1	1:1636:A:LEU:HD22	2	0.82	0.64	0.82
(1,1060)	1:1529:A:LEU:HD22	1:1581:A:LEU:HG	2	0.78	0.42	0.78
(1,1004)	1:1644:A:LEU:HD22	1:1645:A:ALA:H	2	0.68	0.04	0.68
(1,1004)	1:1644:A:LEU:HD23	1:1645:A:ALA:H	2	0.68	0.04	0.68
(1,189)	1:1635:A:THR:H	1:1633:A:THR:HG22	2	0.65	0.28	0.65
(1,189)	1:1635:A:THR:H	1:1633:A:THR:HG23	2	0.65	0.28	0.65
(1,1017)	1:1527:A:PHE:HD2	1:1518:A:VAL:HG21	2	0.64	0.03	0.64
(1,686)	1:1644:A:LEU:HD21	1:1529:A:LEU:HA	2	0.62	0.14	0.62
(1,686)	1:1644:A:LEU:HD22	1:1529:A:LEU:HA	2	0.62	0.14	0.62
(1,1010)	1:1548:A:VAL:HG12	1:1542:A:TYR:HD1	2	0.62	0.49	0.62
(1,1010)	1:1548:A:VAL:HG12	1:1542:A:TYR:HD2	2	0.62	0.49	0.62
(1,433)	1:1610:A:ILE:HD12	1:1610:A:ILE:HB	2	0.59	0.01	0.59
(1,12)	1:1625:A:MET:HE1	1:1620:A:PRO:HD2	2	0.58	0.44	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,12)	1:1625:A:MET:HE1	1:1623:A:ARG:HD2	2	0.58	0.44	0.58
(1,434)	1:1610:A:ILE:HD11	1:1590:A:LEU:HB3	2	0.58	0.04	0.58
(1,434)	1:1610:A:ILE:HD13	1:1590:A:LEU:HB3	2	0.58	0.04	0.58
(1,454)	1:1550:A:MET:HE2	1:1610:A:ILE:HG12	2	0.57	0.04	0.57
(1,81)	1:1512:A:GLU:HG2	1:1511:A:ASN:H	2	0.55	0.37	0.55
(1,81)	1:1512:A:GLU:HG2	1:1515:A:ASP:H	2	0.55	0.37	0.55
(1,1578)	1:1644:A:LEU:H	1:1644:A:LEU:HB2	2	0.55	0.02	0.55
(1,1117)	1:1574:A:VAL:HG23	1:1608:A:SER:HA	2	0.53	0.08	0.53
(1,428)	1:1552:A:ILE:HD11	1:1550:A:MET:HG3	2	0.52	0.39	0.52
(1,428)	1:1552:A:ILE:HD13	1:1550:A:MET:HG3	2	0.52	0.39	0.52
(1,2737)	2:56:B:LEU:H	2:56:B:LEU:HD21	2	0.52	0.1	0.52
(1,2737)	2:56:B:LEU:H	2:56:B:LEU:HD23	2	0.52	0.1	0.52
(1,1992)	1:1523:A:THR:H	1:1521:A:PRO:HG2	2	0.52	0.2	0.52
(1,1992)	1:1523:A:THR:H	1:1521:A:PRO:HG3	2	0.52	0.2	0.52
(1,1200)	1:1584:A:VAL:H	1:1518:A:VAL:HG22	2	0.48	0.16	0.48
(1,2874)	2:17:B:LEU:HD11	2:28:B:PHE:HD1	2	0.46	0.29	0.46
(1,2874)	2:17:B:LEU:HD12	2:28:B:PHE:HD1	2	0.46	0.29	0.46
(1,2826)	2:59:B:TYR:H	2:58:B:THR:HG22	2	0.43	0.03	0.43
(1,2826)	2:59:B:TYR:H	2:58:B:THR:HG21	2	0.43	0.03	0.43
(1,50)	1:1635:A:THR:HG22	1:1609:A:VAL:HB	2	0.42	0.12	0.42
(1,50)	1:1635:A:THR:HG21	1:1609:A:VAL:HB	2	0.42	0.12	0.42
(1,484)	1:1610:A:ILE:HG21	1:1610:A:ILE:HG12	2	0.42	0.02	0.42
(1,484)	1:1610:A:ILE:HG23	1:1610:A:ILE:HG12	2	0.42	0.02	0.42
(1,2241)	1:1527:A:PHE:HD2	1:1519:A:THR:HA	2	0.41	0.29	0.41
(1,2231)	1:1567:A:PHE:HD1	1:1542:A:TYR:HD1	2	0.39	0.09	0.39
(1,2231)	1:1567:A:PHE:HD2	1:1542:A:TYR:HD2	2	0.39	0.09	0.39
(1,2281)	2:42:B:ILE:HD11	2:59:B:TYR:HB3	2	0.38	0.21	0.38
(1,2281)	2:42:B:ILE:HD12	2:59:B:TYR:HB3	2	0.38	0.21	0.38
(1,1770)	1:1547:A:VAL:H	1:1549:A:TYR:HE2	2	0.38	0.22	0.38
(1,1330)	1:1569:A:GLN:H	1:1568:A:GLY:HA2	2	0.36	0.02	0.36
(1,1718)	1:1579:A:LYS:H	1:1578:A:ASN:HB3	2	0.36	0.01	0.36
(1,2494)	2:37:B:ARG:HG2	2:37:B:ARG:HA	2	0.36	0.26	0.36
(1,1342)	1:1535:A:ARG:H	1:1534:A:GLY:HA3	2	0.35	0.07	0.35
(1,397)	1:1636:A:LEU:HD11	2:19:B:PHE:HZ	2	0.34	0.12	0.34
(1,397)	1:1636:A:LEU:HD13	2:19:B:PHE:HZ	2	0.34	0.12	0.34
(1,2506)	2:56:B:LEU:HD11	2:20:B:VAL:H	2	0.34	0.16	0.34
(1,2506)	2:56:B:LEU:HD13	2:20:B:VAL:H	2	0.34	0.16	0.34
(1,1496)	1:1574:A:VAL:H	1:1574:A:VAL:HG13	2	0.34	0.04	0.34
(1,1496)	1:1574:A:VAL:H	1:1574:A:VAL:HG11	2	0.34	0.04	0.34
(1,935)	1:1636:A:LEU:HD11	1:1636:A:LEU:H	2	0.34	0.12	0.34
(1,935)	1:1636:A:LEU:HD13	1:1636:A:LEU:H	2	0.34	0.12	0.34
(1,2378)	2:42:B:ILE:HG22	2:59:B:TYR:HB3	2	0.34	0.01	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2378)	2:42:B:ILE:HG21	2:59:B:TYR:HB3	2	0.34	0.01	0.34
(1,1091)	1:1604:A:LEU:HD21	1:1633:A:THR:HA	2	0.33	0.01	0.33
(1,1091)	1:1604:A:LEU:HD23	1:1633:A:THR:HA	2	0.33	0.01	0.33
(1,538)	1:1570:A:THR:HG23	1:1569:A:GLN:HB3	2	0.32	0.08	0.32
(1,538)	1:1570:A:THR:HG22	1:1569:A:GLN:HB3	2	0.32	0.08	0.32
(1,8)	1:1610:A:ILE:HD13	1:1612:A:PHE:HZ	2	0.31	0.12	0.31
(1,8)	1:1610:A:ILE:HD12	1:1612:A:PHE:HZ	2	0.31	0.12	0.31
(1,365)	2:59:B:TYR:H	2:56:B:LEU:HD12	2	0.31	0.01	0.31
(1,365)	2:59:B:TYR:H	2:56:B:LEU:HD11	2	0.31	0.01	0.31
(1,499)	1:1645:A:ALA:HB3	1:1612:A:PHE:HB2	2	0.31	0.02	0.31
(1,2832)	2:41:B:GLY:H	2:43:B:VAL:HG12	2	0.31	0.01	0.31
(1,2832)	2:41:B:GLY:H	2:43:B:VAL:HG13	2	0.31	0.01	0.31
(1,1130)	1:1554:A:GLY:H	1:1592:A:TYR:HH	2	0.3	0.13	0.3
(1,911)	1:1510:A:SER:HB3	1:1511:A:ASN:H	2	0.3	0.01	0.3
(1,1094)	1:1588:A:LEU:HD12	1:1581:A:LEU:HG	2	0.3	0.11	0.3
(1,1094)	1:1588:A:LEU:HD13	1:1581:A:LEU:HG	2	0.3	0.11	0.3
(1,1782)	1:1517:A:GLN:H	1:1515:A:ASP:HB3	2	0.29	0.07	0.29
(1,1782)	1:1517:A:GLN:H	1:1515:A:ASP:HB2	2	0.29	0.07	0.29
(1,1904)	1:1517:A:GLN:HE21	1:1517:A:GLN:HG2	2	0.28	0.0	0.28
(1,2686)	2:6:B:GLU:H	2:6:B:GLU:HG2	2	0.28	0.02	0.28
(1,19)	1:1618:A:ALA:HB1	1:1643:A:PRO:HB3	2	0.27	0.17	0.27
(1,19)	1:1618:A:ALA:HB2	1:1617:A:GLU:HB2	2	0.27	0.17	0.27
(1,63)	1:1526:A:LEU:HD22	1:1517:A:GLN:HG3	2	0.26	0.08	0.26
(1,63)	1:1526:A:LEU:HD21	1:1517:A:GLN:HG3	2	0.26	0.08	0.26
(1,579)	1:1519:A:THR:HG21	1:1525:A:HIS:H	2	0.26	0.02	0.26
(1,36)	1:1540:A:ALA:HB1	1:1548:A:VAL:H	2	0.26	0.01	0.26
(1,36)	1:1540:A:ALA:HB2	1:1548:A:VAL:H	2	0.26	0.01	0.26
(1,748)	1:1513:A:HIS:HB2	1:1512:A:GLU:HA	2	0.25	0.07	0.25
(1,748)	1:1513:A:HIS:HB3	1:1512:A:GLU:HA	2	0.25	0.07	0.25
(1,1331)	1:1569:A:GLN:HG2	1:1569:A:GLN:H	2	0.25	0.07	0.25
(1,114)	1:1542:A:TYR:HE2	1:1629:A:LEU:HB2	2	0.24	0.04	0.24
(1,114)	1:1542:A:TYR:HE1	1:1629:A:LEU:HB2	2	0.24	0.04	0.24
(1,172)	1:1513:A:HIS:H	1:1514:A:ASP:HB2	2	0.24	0.08	0.24
(1,2552)	2:25:B:GLY:H	2:61:B:ALA:HB1	2	0.24	0.05	0.24
(1,2947)	2:19:B:PHE:HD1	2:20:B:VAL:HA	2	0.22	0.05	0.22
(1,410)	1:1543:A:SER:HB2	1:1546:A:GLY:H	2	0.22	0.09	0.22
(1,410)	1:1543:A:SER:HB2	1:1547:A:VAL:H	2	0.22	0.09	0.22
(1,315)	2:32:B:ALA:H	2:31:B:PRO:HG3	2	0.22	0.07	0.22
(1,665)	1:1563:A:VAL:HG21	1:1566:A:CYS:HB3	2	0.22	0.08	0.22
(1,2135)	1:1637:A:PHE:H	1:1627:A:ILE:HG12	2	0.22	0.04	0.22
(1,955)	1:1574:A:VAL:HG11	1:1567:A:PHE:HD1	2	0.21	0.04	0.21
(1,955)	1:1574:A:VAL:HG12	1:1567:A:PHE:HD1	2	0.21	0.04	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,977)	1:1508:A:MET:HE3	1:1508:A:MET:HA	2	0.21	0.1	0.21
(1,2540)	2:50:B:SER:H	2:49:B:ARG:HB2	2	0.21	0.08	0.21
(1,2038)	1:1567:A:PHE:H	1:1567:A:PHE:HE2	2	0.2	0.03	0.2
(1,2685)	2:6:B:GLU:H	2:5:B:SER:HA	2	0.2	0.03	0.2
(1,1120)	1:1526:A:LEU:HB3	1:1526:A:LEU:H	2	0.2	0.01	0.2
(1,2721)	2:8:B:LEU:H	2:8:B:LEU:HD21	2	0.2	0.09	0.2
(1,2721)	2:8:B:LEU:H	2:8:B:LEU:HD22	2	0.2	0.09	0.2
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB1	2	0.19	0.02	0.19
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB2	2	0.19	0.02	0.19
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB3	2	0.19	0.02	0.19
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB1	2	0.19	0.02	0.19
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB2	2	0.19	0.02	0.19
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB3	2	0.19	0.02	0.19
(1,2831)	2:41:B:GLY:H	2:42:B:ILE:HG12	2	0.18	0.02	0.18
(1,1925)	1:1575:A:GLY:H	1:1595:A:GLY:HA2	2	0.18	0.04	0.18
(1,485)	1:1577:A:ALA:HB3	1:1564:A:GLY:HA3	2	0.18	0.04	0.18
(1,1710)	1:1632:A:GLN:H	1:1631:A:LYS:HB2	2	0.18	0.04	0.18
(1,2621)	2:37:B:ARG:H	2:37:B:ARG:HD3	2	0.18	0.03	0.18
(1,2621)	2:37:B:ARG:H	2:37:B:ARG:HD2	2	0.18	0.03	0.18
(1,2928)	2:59:B:TYR:H	2:59:B:TYR:HB3	2	0.18	0.0	0.18
(1,1280)	1:1618:A:ALA:H	1:1617:A:GLU:HB2	2	0.17	0.0	0.17
(1,1471)	1:1551:A:SER:H	1:1550:A:MET:HG2	2	0.17	0.04	0.17
(1,2053)	1:1573:A:SER:H	1:1563:A:VAL:HG21	2	0.17	0.02	0.17
(1,1333)	1:1569:A:GLN:H	1:1568:A:GLY:H	2	0.16	0.06	0.16
(1,1901)	1:1545:A:SER:H	1:1544:A:LYS:HD2	2	0.16	0.01	0.16
(1,2991)	2:42:B:ILE:HG22	2:59:B:TYR:HE2	2	0.16	0.02	0.16
(1,2991)	2:42:B:ILE:HG23	2:59:B:TYR:HE1	2	0.16	0.02	0.16
(1,2581)	2:32:B:ALA:H	2:32:B:ALA:HB1	2	0.16	0.01	0.16
(1,2581)	2:32:B:ALA:H	2:32:B:ALA:HB2	2	0.16	0.01	0.16
(1,509)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD21	2	0.15	0.03	0.15
(1,549)	1:1574:A:VAL:HG23	1:1636:A:LEU:HB2	2	0.15	0.03	0.15
(1,549)	1:1574:A:VAL:HG21	1:1636:A:LEU:HB2	2	0.15	0.03	0.15
(1,1625)	1:1509:A:LYS:HA	1:1510:A:SER:H	2	0.15	0.03	0.15
(1,582)	1:1540:A:ALA:HB1	1:1548:A:VAL:H	2	0.14	0.01	0.14
(1,582)	1:1540:A:ALA:HB2	1:1548:A:VAL:H	2	0.14	0.01	0.14
(1,1975)	1:1538:A:PHE:H	1:1538:A:PHE:HD1	2	0.14	0.04	0.14
(1,1975)	1:1538:A:PHE:H	1:1538:A:PHE:HD2	2	0.14	0.04	0.14
(1,2029)	1:1563:A:VAL:H	1:1561:A:PRO:HB3	2	0.14	0.01	0.14
(1,2079)	1:1588:A:LEU:HD11	1:1583:A:TYR:H	2	0.14	0.04	0.14
(1,2079)	1:1588:A:LEU:HD12	1:1583:A:TYR:H	2	0.14	0.04	0.14
(1,2514)	2:13:B:LEU:HD23	2:13:B:LEU:HA	2	0.14	0.02	0.14
(1,2514)	2:13:B:LEU:HD22	2:13:B:LEU:HA	2	0.14	0.02	0.14

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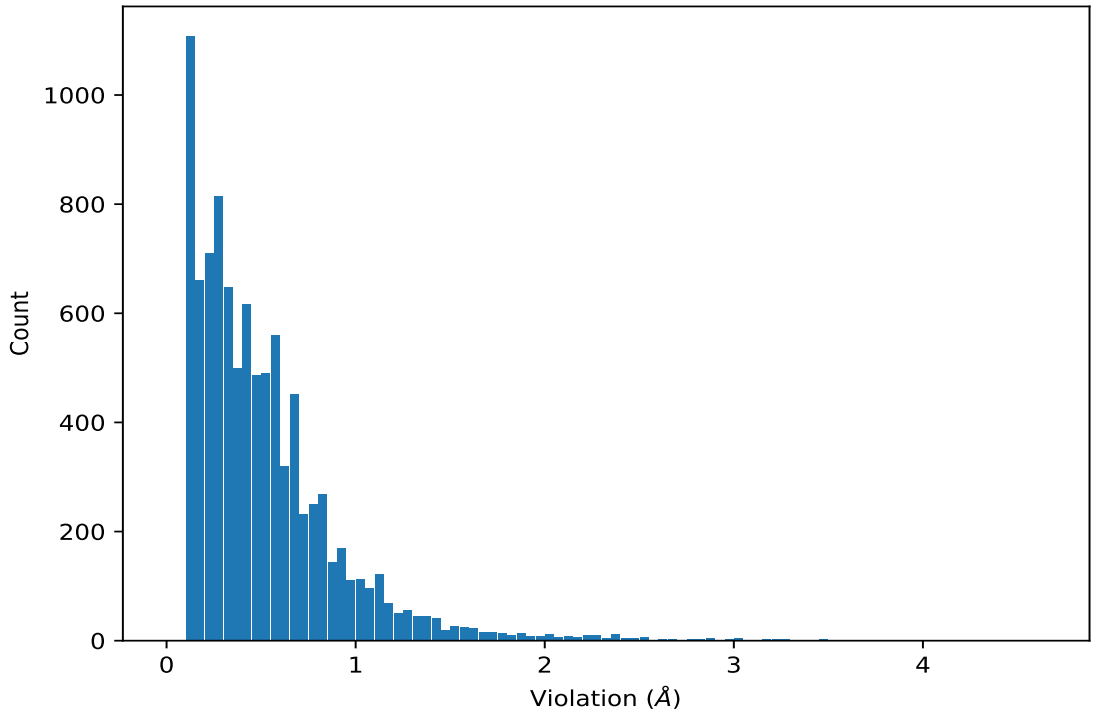
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,858)	1:1647:A:GLU:HA	1:1648:A:PRO:HD3	2	0.13	0.01	0.13
(1,2772)	2:66:B:SER:H	2:65:B:LYS:HA	2	0.13	0.01	0.13
(1,562)	1:1532:A:LEU:HD22	1:1640:A:TRP:HZ2	2	0.12	0.01	0.12
(1,562)	1:1532:A:LEU:HD23	1:1640:A:TRP:HZ2	2	0.12	0.01	0.12
(1,1818)	1:1632:A:GLN:HG2	1:1632:A:GLN:HE21	2	0.12	0.01	0.12
(1,1818)	1:1632:A:GLN:HG3	1:1632:A:GLN:HE21	2	0.12	0.01	0.12
(1,2597)	2:33:B:SER:H	2:35:B:VAL:H	2	0.12	0.02	0.12
(1,1165)	1:1610:A:ILE:H	1:1591:A:VAL:HA	2	0.12	0.0	0.12
(1,2639)	2:38:B:ARG:H	2:32:B:ALA:HA	2	0.12	0.0	0.12
(1,2864)	2:51:B:CYS:H	2:52:B:ASP:HA	2	0.12	0.0	0.12
(1,2886)	2:28:B:PHE:H	2:29:B:SER:H	2	0.12	0.0	0.12
(1,750)	1:1617:A:GLU:HB2	1:1618:A:ALA:H	2	0.11	0.0	0.11
(1,990)	1:1636:A:LEU:HD12	1:1636:A:LEU:HB3	2	0.11	0.0	0.11
(1,2391)	2:6:B:GLU:H	2:5:B:SER:HB2	2	0.11	0.0	0.11
(1,644)	1:1526:A:LEU:HD13	1:1526:A:LEU:H	2	0.11	0.0	0.11
(1,644)	1:1526:A:LEU:HD12	1:1526:A:LEU:H	2	0.11	0.0	0.11
(1,2309)	2:64:B:ALA:H	2:63:B:PRO:HB3	2	0.11	0.0	0.11
(1,435)	1:1610:A:ILE:HD12	1:1610:A:ILE:HG13	2	0.1	0.0	0.1
(1,435)	1:1610:A:ILE:HD11	1:1610:A:ILE:HG13	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	17	4.61
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD2	5	4.56
(1,2504)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	2	4.31
(1,2450)	2:55:B:LEU:HD12	2:58:B:THR:HG23	15	4.03
(1,2537)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	2	3.94
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	20	3.71
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	15	3.65
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	14	3.57
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD13	2	3.51
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD11	11	3.49
(1,1089)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	20	3.46
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	15	3.41
(1,1449)	1:1589:A:GLN:H	1:1584:A:VAL:HG21	11	3.37
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	4	3.31
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	13	3.29
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD12	7	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	20	3.24
(1,2961)	2:56:B:LEU:HD23	2:53:B:LEU:H	7	3.21
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	9	3.18
(1,1089)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	5	3.17
(1,275)	2:13:B:LEU:HD22	2:8:B:LEU:HA	1	3.09
(1,1449)	1:1589:A:GLN:H	1:1584:A:VAL:HG23	5	3.04
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	16	3.04
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	12	3.03
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD21	8	3.02
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD3	17	3.01
(1,1449)	1:1589:A:GLN:H	1:1584:A:VAL:HG21	3	2.98
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	12	2.96
(1,691)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	5	2.96
(1,2502)	2:56:B:LEU:HD23	2:53:B:LEU:H	7	2.94
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD13	18	2.89
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	5	2.88
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD21	7	2.87
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD23	15	2.87
(1,722)	1:1581:A:LEU:HD13	1:1518:A:VAL:HB	1	2.86
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	6	2.83
(1,2301)	2:20:B:VAL:HG13	2:60:B:CYS:HB2	4	2.82
(1,650)	1:1590:A:LEU:HD21	1:1581:A:LEU:H	5	2.8
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG22	14	2.77
(1,270)	2:59:B:TYR:H	2:56:B:LEU:HD22	11	2.75
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	1	2.72
(1,3009)	2:56:B:LEU:HD23	2:17:B:LEU:HD23	20	2.67
(1,2537)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	12	2.67
(1,696)	1:1644:A:LEU:HD21	1:1529:A:LEU:HD23	5	2.61
(1,230)	2:55:B:LEU:HD11	2:59:B:TYR:H	15	2.61
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	7	2.6
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG22	7	2.55
(1,696)	1:1644:A:LEU:HD23	1:1529:A:LEU:HD22	20	2.55
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	1	2.54
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	4	2.54
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	11	2.52
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	16	2.51
(1,700)	1:1590:A:LEU:HD21	1:1581:A:LEU:HA	5	2.49
(1,1058)	1:1626:A:LEU:HD23	1:1638:A:PHE:HD1	18	2.47
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	7	2.46
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	13	2.45
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	7	2.44
(1,577)	1:1529:A:LEU:HD23	1:1528:A:ASP:H	14	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	8	2.42
(1,1024)	1:1552:A:ILE:HD12	1:1590:A:LEU:HD11	5	2.41
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	7	2.4
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	17	2.4
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	15	2.39
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD21	15	2.39
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	17	2.38
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	18	2.38
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD13	11	2.37
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	12	2.37
(1,142)	1:1581:A:LEU:HD11	1:1582:A:ARG:HG3	1	2.37
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	4	2.35
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	5	2.35
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	20	2.33
(1,271)	2:54:B:ALA:HB2	2:56:B:LEU:HD21	8	2.33
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	12	2.32
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	4	2.32
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	8	2.3
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD23	5	2.3
(1,218)	1:1567:A:PHE:H	1:1548:A:VAL:HG13	5	2.29
(1,1075)	1:1581:A:LEU:HD23	1:1590:A:LEU:HD12	1	2.28
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	18	2.28
(1,218)	1:1567:A:PHE:H	1:1548:A:VAL:HG11	12	2.28
(1,2303)	2:20:B:VAL:HG21	2:19:B:PHE:HE2	13	2.27
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG11	16	2.26
(1,2276)	2:14:B:VAL:HG22	2:28:B:PHE:HE1	7	2.25
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD11	6	2.25
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	19	2.24
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	11	2.24
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	10	2.23
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	20	2.23
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD22	11	2.23
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	9	2.21
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD22	19	2.21
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	2	2.2
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	2	2.2
(1,226)	2:17:B:LEU:HD11	2:18:B:GLN:HA	6	2.2
(1,2537)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	1	2.17
(1,2301)	2:20:B:VAL:HG13	2:60:B:CYS:HB2	9	2.17
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	5	2.17
(1,2276)	2:14:B:VAL:HG21	2:28:B:PHE:HE2	2	2.16
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	10	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	16	2.15
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	15	2.13
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	2	2.12
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	3	2.12
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	13	2.12
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD21	17	2.12
(1,55)	1:1518:A:VAL:HG12	1:1511:A:ASN:HB2	5	2.12
(1,2298)	2:55:B:LEU:HD11	2:56:B:LEU:HA	15	2.11
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	15	2.11
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	18	2.1
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD22	15	2.08
(1,1084)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD21	16	2.08
(1,2301)	2:20:B:VAL:HG11	2:60:B:CYS:HB2	13	2.07
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD22	18	2.07
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	8	2.06
(1,271)	2:54:B:ALA:HB2	2:56:B:LEU:HD22	4	2.06
(1,271)	2:54:B:ALA:HB3	2:56:B:LEU:HD23	15	2.06
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	10	2.05
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	11	2.04
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	4	2.03
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	11	2.02
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	12	2.02
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE2	4	2.02
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	10	2.01
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	1	2.01
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	13	2.01
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	8	2.0
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	5	2.0
(1,1084)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	18	1.99
(1,657)	1:1581:A:LEU:HD13	1:1582:A:ARG:HA	1	1.99
(1,3009)	2:56:B:LEU:HD21	2:17:B:LEU:HD23	5	1.98
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	7	1.98
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	16	1.97
(1,2303)	2:20:B:VAL:HG21	2:19:B:PHE:HE2	9	1.97
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	9	1.96
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	6	1.96
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	12	1.96
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD11	1	1.95
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD21	17	1.95
(1,2527)	2:58:B:THR:HG21	2:59:B:TYR:HB3	6	1.94
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	14	1.94
(1,2276)	2:14:B:VAL:HG23	2:28:B:PHE:HE1	11	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD12	7	1.93
(1,226)	2:17:B:LEU:HD11	2:18:B:GLN:HA	8	1.92
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD12	12	1.92
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD12	3	1.91
(1,951)	1:1627:A:ILE:HA	1:1626:A:LEU:HD13	18	1.9
(1,2527)	2:58:B:THR:HG22	2:59:B:TYR:HB3	2	1.88
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	11	1.88
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	11	1.87
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	13	1.87
(1,544)	1:1518:A:VAL:HG23	1:1517:A:GLN:HA	5	1.87
(1,237)	2:20:B:VAL:HG22	2:26:B:PHE:HD2	4	1.87
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	5	1.86
(1,937)	1:1636:A:LEU:HD22	1:1542:A:TYR:HE2	16	1.86
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	6	1.85
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	17	1.85
(1,666)	1:1626:A:LEU:HD21	1:1636:A:LEU:HD23	16	1.85
(1,174)	1:1513:A:HIS:H	1:1518:A:VAL:HG11	5	1.85
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	12	1.84
(1,271)	2:54:B:ALA:HB1	2:53:B:LEU:HD12	1	1.84
(1,2456)	2:35:B:VAL:H	2:35:B:VAL:HG21	10	1.83
(1,564)	1:1591:A:VAL:HG21	1:1593:A:LYS:H	18	1.82
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	13	1.82
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	13	1.81
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	2	1.8
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	19	1.8
(1,1202)	1:1584:A:VAL:H	1:1584:A:VAL:HG23	11	1.8
(1,564)	1:1591:A:VAL:HG21	1:1593:A:LYS:H	3	1.8
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	15	1.79
(1,564)	1:1591:A:VAL:HG23	1:1593:A:LYS:H	8	1.79
(1,564)	1:1591:A:VAL:HG21	1:1593:A:LYS:H	17	1.79
(1,231)	2:55:B:LEU:HD22	2:57:B:GLU:H	15	1.79
(1,1116)	1:1626:A:LEU:HD22	1:1638:A:PHE:HZ	18	1.78
(1,14)	1:1552:A:ILE:HG22	1:1532:A:LEU:HD23	14	1.78
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	15	1.76
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	12	1.75
(1,694)	1:1636:A:LEU:HD13	1:1635:A:THR:HA	12	1.75
(1,666)	1:1626:A:LEU:HD22	1:1636:A:LEU:HD23	18	1.75
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	15	1.75
(1,271)	2:54:B:ALA:HB1	2:56:B:LEU:HD23	6	1.75
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	7	1.75
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	10	1.74
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG11	16	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD12	20	1.74
(1,3010)	2:17:B:LEU:HD21	2:56:B:LEU:HD12	17	1.73
(1,187)	1:1567:A:PHE:H	1:1565:A:ALA:HB3	4	1.73
(1,3010)	2:17:B:LEU:HD23	2:56:B:LEU:HD13	5	1.72
(1,2232)	1:1567:A:PHE:HD1	1:1606:A:TYR:HE1	5	1.72
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	20	1.72
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG22	11	1.72
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	10	1.72
(1,237)	2:20:B:VAL:HG23	2:26:B:PHE:HD2	9	1.72
(1,55)	1:1518:A:VAL:HG13	1:1511:A:ASN:HB3	12	1.72
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	2	1.71
(1,482)	1:1552:A:ILE:HG22	1:1590:A:LEU:HD11	5	1.71
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG12	10	1.71
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD22	12	1.71
(1,3010)	2:17:B:LEU:HD23	2:56:B:LEU:HD13	20	1.7
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	2	1.7
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD12	14	1.7
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	6	1.69
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG23	17	1.69
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD22	14	1.69
(1,1358)	1:1581:A:LEU:HD12	1:1582:A:ARG:H	1	1.68
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	1	1.68
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD22	9	1.68
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	2	1.68
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG13	7	1.67
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG21	18	1.67
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	15	1.67
(1,115)	1:1574:A:VAL:HG21	1:1566:A:CYS:H	14	1.67
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG23	12	1.66
(1,450)	1:1550:A:MET:HE3	1:1548:A:VAL:HG22	19	1.66
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE1	8	1.65
(1,2232)	1:1567:A:PHE:HD1	1:1606:A:TYR:HE1	13	1.65
(1,2961)	2:56:B:LEU:HD23	2:53:B:LEU:H	11	1.64
(1,1747)	1:1567:A:PHE:H	1:1574:A:VAL:HG12	7	1.64
(1,1202)	1:1584:A:VAL:H	1:1584:A:VAL:HG22	5	1.64
(1,226)	2:17:B:LEU:HD13	2:57:B:GLU:HA	5	1.64
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD23	12	1.63
(1,2294)	2:17:B:LEU:HD22	2:16:B:THR:H	8	1.63
(1,1450)	1:1589:A:GLN:H	1:1581:A:LEU:HD12	1	1.63
(1,647)	1:1529:A:LEU:HD13	1:1612:A:PHE:HE2	14	1.63
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG13	14	1.63
(1,2186)	1:1556:A:ASN:HD22	1:1537:A:GLY:HA2	12	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	5	1.62
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	5	1.62
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG13	13	1.62
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	9	1.61
(1,1202)	1:1584:A:VAL:H	1:1584:A:VAL:HG23	3	1.61
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	15	1.61
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	7	1.6
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	18	1.6
(1,1747)	1:1567:A:PHE:H	1:1574:A:VAL:HG11	14	1.6
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	20	1.6
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	18	1.59
(1,715)	1:1604:A:LEU:HD22	1:1603:A:GLY:HA2	6	1.59
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG11	3	1.59
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG13	6	1.59
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	12	1.59
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB2	14	1.59
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD23	10	1.59
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	8	1.58
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	4	1.58
(1,2213)	1:1528:A:ASP:H	1:1529:A:LEU:HD23	14	1.58
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG11	1	1.58
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	6	1.58
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	11	1.58
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	9	1.57
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	12	1.57
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	18	1.56
(1,2293)	2:17:B:LEU:HD11	2:56:B:LEU:HD11	7	1.56
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD22	4	1.56
(1,715)	1:1604:A:LEU:HD13	1:1603:A:GLY:HA2	20	1.56
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	20	1.56
(1,49)	1:1565:A:ALA:HB3	1:1556:A:ASN:HB3	1	1.56
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	16	1.56
(1,3009)	2:42:B:ILE:HG23	2:17:B:LEU:HD21	17	1.55
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD21	15	1.55
(1,695)	1:1529:A:LEU:HD11	1:1644:A:LEU:HD21	20	1.55
(1,2277)	2:42:B:ILE:HD11	2:45:B:GLU:HB2	18	1.54
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	13	1.54
(1,729)	1:1590:A:LEU:HD13	1:1552:A:ILE:HA	5	1.54
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	2	1.54
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	10	1.54
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	6	1.53
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD12	18	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:1608:A:SER:HA	1:1636:A:LEU:HD22	5	1.53
(1,715)	1:1604:A:LEU:HD11	1:1603:A:GLY:HA2	17	1.53
(1,544)	1:1518:A:VAL:HG23	1:1517:A:GLN:HA	12	1.53
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	13	1.53
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	14	1.53
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	1	1.52
(1,1190)	1:1549:A:TYR:H	1:1548:A:VAL:HG22	4	1.52
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	15	1.52
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	6	1.52
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	9	1.52
(1,267)	2:35:B:VAL:HG21	2:37:B:ARG:HD3	10	1.52
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD21	4	1.52
(1,5)	1:1552:A:ILE:HD11	1:1532:A:LEU:HD23	14	1.52
(1,2294)	2:17:B:LEU:HD22	2:16:B:THR:H	6	1.51
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	9	1.51
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD3	6	1.51
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD12	7	1.5
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	7	1.5
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	14	1.5
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	8	1.5
(1,2846)	2:17:B:LEU:HD12	2:26:B:PHE:HD2	20	1.49
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	20	1.49
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	5	1.49
(1,1053)	1:1574:A:VAL:HG21	1:1565:A:ALA:HB2	14	1.49
(1,450)	1:1550:A:MET:HE2	1:1548:A:VAL:HG23	8	1.49
(1,2482)	2:13:B:LEU:HD11	2:12:B:GLU:HB3	1	1.48
(1,715)	1:1604:A:LEU:HD13	1:1603:A:GLY:HA2	7	1.48
(1,715)	1:1604:A:LEU:HD13	1:1603:A:GLY:HA2	14	1.48
(1,643)	1:1604:A:LEU:HD13	1:1633:A:THR:H	1	1.48
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB2	13	1.48
(1,232)	2:55:B:LEU:HD13	2:49:B:ARG:HD3	15	1.48
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD11	6	1.47
(1,115)	1:1574:A:VAL:HG21	1:1566:A:CYS:H	7	1.47
(1,3015)	1:1636:A:LEU:HD22	2:19:B:PHE:HE2	16	1.46
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	3	1.46
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	7	1.46
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	17	1.46
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	18	1.46
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	4	1.46
(1,239)	2:18:B:GLN:H	2:20:B:VAL:HG11	13	1.46
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	19	1.45
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD11	11	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD11	15	1.45
(1,971)	1:1608:A:SER:HA	1:1636:A:LEU:HD23	4	1.45
(1,658)	1:1590:A:LEU:HD21	1:1590:A:LEU:HA	5	1.45
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	19	1.45
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	3	1.45
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	7	1.44
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	19	1.44
(1,1053)	1:1574:A:VAL:HG21	1:1565:A:ALA:HB3	7	1.44
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD11	1	1.44
(1,505)	1:1618:A:ALA:HB1	1:1616:A:PRO:HD2	10	1.44
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB3	2	1.44
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	17	1.44
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	1	1.44
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	2	1.44
(1,174)	1:1511:A:ASN:H	1:1518:A:VAL:HG11	12	1.44
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD21	13	1.44
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	11	1.43
(1,2302)	2:20:B:VAL:HG11	2:17:B:LEU:HA	4	1.43
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	20	1.43
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	5	1.43
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	17	1.43
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	11	1.43
(1,697)	1:1644:A:LEU:HD12	1:1529:A:LEU:HD11	14	1.43
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	7	1.43
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD11	18	1.43
(1,695)	1:1529:A:LEU:HD12	1:1644:A:LEU:HD22	5	1.42
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD22	15	1.42
(1,505)	1:1618:A:ALA:HB3	1:1616:A:PRO:HD2	8	1.42
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	18	1.42
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	20	1.42
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	5	1.42
(1,11)	1:1625:A:MET:HE3	1:1626:A:LEU:HA	11	1.42
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD1	9	1.41
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	9	1.41
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD11	1	1.41
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	13	1.41
(1,505)	1:1618:A:ALA:HB3	1:1616:A:PRO:HD2	1	1.41
(1,450)	1:1550:A:MET:HE1	1:1548:A:VAL:HG11	9	1.41
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	18	1.41
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD2	17	1.4
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD2	2	1.4
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	20	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:1591:A:VAL:HG23	1:1607:A:LYS:HD3	8	1.4
(1,715)	1:1604:A:LEU:HD12	1:1603:A:GLY:HA2	18	1.4
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	14	1.4
(1,563)	1:1591:A:VAL:HG12	1:1589:A:GLN:HE21	4	1.4
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	2	1.4
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	9	1.4
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	12	1.4
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	17	1.4
(1,2326)	2:32:B:ALA:HB1	2:31:B:PRO:HD3	9	1.39
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	12	1.39
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	15	1.39
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	6	1.39
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	13	1.39
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB2	14	1.39
(1,93)	1:1565:A:ALA:HA	1:1548:A:VAL:HG21	4	1.39
(1,49)	1:1565:A:ALA:HB1	1:1556:A:ASN:HB3	19	1.39
(1,505)	1:1618:A:ALA:HB1	1:1616:A:PRO:HD2	11	1.38
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	20	1.38
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	5	1.37
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	16	1.37
(1,2292)	2:17:B:LEU:HD11	2:20:B:VAL:HG11	7	1.37
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	9	1.37
(1,985)	1:1601:A:LYS:HB3	1:1600:A:SER:HB2	19	1.37
(1,563)	1:1591:A:VAL:HG12	1:1589:A:GLN:HE21	14	1.37
(1,505)	1:1618:A:ALA:HB1	1:1616:A:PRO:HD2	12	1.37
(1,2868)	2:17:B:LEU:HD12	2:28:B:PHE:HD1	20	1.36
(1,2502)	2:56:B:LEU:HD23	2:53:B:LEU:H	11	1.36
(1,2292)	2:17:B:LEU:HD13	2:42:B:ILE:HG13	9	1.36
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	20	1.36
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	2	1.36
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	5	1.36
(1,87)	1:1584:A:VAL:HG13	1:1585:A:ASP:HB2	16	1.36
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG11	18	1.35
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	7	1.35
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	7	1.35
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	9	1.35
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	19	1.35
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	13	1.35
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	10	1.35
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	14	1.35
(1,325)	2:17:B:LEU:HD12	2:14:B:VAL:HA	15	1.35
(1,2846)	2:17:B:LEU:HD12	2:26:B:PHE:HD1	5	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD1	4	1.34
(1,1673)	1:1530:A:SER:H	1:1529:A:LEU:HD22	14	1.34
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	14	1.34
(1,563)	1:1591:A:VAL:HG12	1:1589:A:GLN:HE21	1	1.34
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	13	1.34
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	4	1.34
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG22	8	1.34
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD21	13	1.34
(1,87)	1:1587:A:VAL:HG13	1:1612:A:PHE:HB3	12	1.34
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	13	1.34
(1,2232)	1:1567:A:PHE:HD1	1:1606:A:TYR:HE1	18	1.33
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	9	1.33
(1,726)	1:1604:A:LEU:HD13	1:1602:A:SER:HA	17	1.33
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	20	1.33
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	6	1.33
(1,56)	1:1563:A:VAL:HG21	1:1559:A:CYS:H	7	1.33
(1,56)	1:1563:A:VAL:HG22	1:1572:A:ILE:H	14	1.33
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD11	2	1.33
(1,2437)	2:56:B:LEU:HD13	2:17:B:LEU:HA	7	1.32
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG22	13	1.32
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	7	1.32
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	7	1.32
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	18	1.32
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	20	1.32
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	2	1.32
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	12	1.32
(1,613)	1:1574:A:VAL:HG11	1:1565:A:ALA:HB2	19	1.32
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	4	1.32
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	8	1.32
(1,2860)	2:17:B:LEU:HD12	2:28:B:PHE:HE1	20	1.31
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD22	2	1.31
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG21	17	1.31
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	17	1.31
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	3	1.31
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	2	1.31
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	1	1.31
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD11	3	1.31
(1,1591)	1:1518:A:VAL:H	1:1518:A:VAL:HG21	12	1.3
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	18	1.3
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD13	10	1.3
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	16	1.3
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD21	14	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	2	1.3
(1,39)	1:1548:A:VAL:HG23	1:1542:A:TYR:HE2	4	1.3
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD12	3	1.29
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD11	4	1.29
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG12	15	1.29
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	15	1.29
(1,1591)	1:1518:A:VAL:H	1:1518:A:VAL:HG21	5	1.29
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	17	1.29
(1,619)	1:1626:A:LEU:HD21	1:1629:A:LEU:HD12	16	1.29
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	4	1.29
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD23	19	1.29
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	11	1.29
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	8	1.29
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG11	5	1.29
(1,87)	1:1584:A:VAL:HG13	1:1585:A:ASP:HB2	4	1.29
(1,87)	1:1587:A:VAL:HG13	1:1612:A:PHE:HB3	7	1.29
(1,87)	1:1587:A:VAL:HG13	1:1612:A:PHE:HB3	14	1.29
(1,3007)	2:17:B:LEU:H	2:56:B:LEU:HD13	7	1.28
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD11	2	1.28
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	19	1.28
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG12	6	1.28
(1,1040)	1:1591:A:VAL:HG22	1:1607:A:LYS:HD3	3	1.28
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB3	17	1.28
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	12	1.28
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB1	9	1.28
(1,372)	1:1569:A:GLN:HG3	2:15:B:ASP:HB3	17	1.28
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	17	1.28
(1,2508)	2:14:B:VAL:HG21	2:17:B:LEU:HD11	14	1.27
(1,2322)	2:32:B:ALA:HB3	2:33:B:SER:HB3	14	1.27
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	15	1.27
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	15	1.27
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	10	1.27
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	2	1.27
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE2	7	1.27
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	19	1.27
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD22	8	1.26
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	13	1.26
(1,1417)	1:1591:A:VAL:H	1:1590:A:LEU:HD23	5	1.26
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	1	1.26
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	5	1.26
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	10	1.26
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB2	16	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE1	16	1.26
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	11	1.26
(1,390)	2:19:B:PHE:HE2	1:1636:A:LEU:HD22	16	1.26
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	1	1.26
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	2	1.26
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	3	1.26
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	15	1.26
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	7	1.26
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD13	3	1.25
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	8	1.25
(1,586)	1:1548:A:VAL:HG22	1:1638:A:PHE:HD1	18	1.25
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	13	1.25
(1,505)	1:1618:A:ALA:HB1	1:1616:A:PRO:HD2	3	1.25
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	8	1.25
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	12	1.25
(1,237)	2:20:B:VAL:HG23	2:26:B:PHE:HD2	13	1.25
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	12	1.24
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD2	15	1.24
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG21	7	1.24
(1,2302)	2:20:B:VAL:HG11	2:17:B:LEU:HA	9	1.24
(1,2302)	2:20:B:VAL:HG11	2:17:B:LEU:HA	13	1.24
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	9	1.24
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	9	1.24
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG11	17	1.24
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	6	1.24
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	6	1.24
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	8	1.24
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	8	1.24
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	19	1.24
(1,2482)	2:13:B:LEU:HD11	2:12:B:GLU:HB3	12	1.23
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	16	1.23
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG12	14	1.23
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG11	20	1.23
(1,818)	1:1606:A:TYR:HB3	1:1596:A:SER:H	12	1.23
(1,709)	1:1590:A:LEU:HD11	1:1612:A:PHE:HZ	5	1.23
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG21	2	1.23
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	5	1.23
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	10	1.23
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	10	1.22
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	3	1.22
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	5	1.22
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB3	9	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:1574:A:VAL:HG12	1:1565:A:ALA:HB2	18	1.22
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	17	1.22
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	18	1.22
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	8	1.22
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	16	1.22
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD11	3	1.22
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	8	1.21
(2,1)	1:1574:A:VAL:HG23	1:1636:A:LEU:H	10	1.21
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD12	4	1.21
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	15	1.21
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	12	1.21
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	8	1.21
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	10	1.21
(1,2232)	1:1567:A:PHE:HD2	1:1542:A:TYR:HE2	14	1.21
(1,1066)	1:1588:A:LEU:HD13	1:1518:A:VAL:HG12	3	1.21
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG12	8	1.21
(1,1060)	1:1529:A:LEU:HD22	1:1581:A:LEU:HG	14	1.21
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	5	1.21
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD13	12	1.21
(1,536)	1:1609:A:VAL:HG22	1:1607:A:LYS:HE3	10	1.21
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	9	1.21
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	9	1.21
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	12	1.21
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	18	1.21
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD13	9	1.21
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD13	5	1.2
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	10	1.2
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD13	13	1.2
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	13	1.2
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	19	1.2
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	7	1.2
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	16	1.2
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	1	1.2
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	2	1.2
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB3	20	1.2
(1,325)	2:17:B:LEU:HD11	2:28:B:PHE:HB2	3	1.2
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	7	1.2
(1,267)	2:35:B:VAL:HG23	2:34:B:ARG:HD2	17	1.2
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG11	9	1.2
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	15	1.2
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD11	17	1.19
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG13	3	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	10	1.19
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG13	7	1.19
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD2	4	1.19
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	17	1.19
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	19	1.19
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD12	7	1.19
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD13	13	1.19
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	20	1.18
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	17	1.18
(1,2294)	2:17:B:LEU:HD22	2:16:B:THR:H	5	1.18
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	18	1.18
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	4	1.18
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	1	1.18
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG13	15	1.18
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG13	16	1.18
(1,889)	1:1544:A:LYS:HA	1:1544:A:LYS:HD2	3	1.18
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	14	1.18
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	11	1.18
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	7	1.18
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD22	11	1.18
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	2	1.18
(1,47)	1:1518:A:VAL:HG13	1:1520:A:ASN:HB3	12	1.18
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	8	1.18
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	16	1.18
(2,1)	1:1574:A:VAL:HG23	1:1636:A:LEU:H	17	1.17
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD1	11	1.17
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD23	1	1.17
(1,2322)	2:32:B:ALA:HB2	2:33:B:SER:HB3	17	1.17
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	8	1.17
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	11	1.17
(1,971)	1:1608:A:SER:HA	1:1636:A:LEU:HD23	12	1.17
(1,889)	1:1544:A:LYS:HA	1:1544:A:LYS:HD2	10	1.17
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	1	1.17
(1,248)	2:36:B:SER:HB2	2:30:B:ARG:HG3	12	1.17
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	17	1.17
(1,85)	1:1584:A:VAL:HG23	1:1589:A:GLN:HB3	5	1.17
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	17	1.17
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	1	1.17
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	11	1.17
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	15	1.16
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD12	15	1.16
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	4	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	15	1.16
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	13	1.16
(1,613)	1:1574:A:VAL:HG11	1:1565:A:ALA:HB2	11	1.16
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	14	1.16
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG12	11	1.16
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	9	1.16
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	9	1.16
(1,40)	1:1587:A:VAL:HG21	1:1589:A:GLN:HE21	4	1.16
(1,11)	1:1625:A:MET:HE3	1:1626:A:LEU:HA	1	1.16
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	9	1.16
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD21	20	1.15
(1,2326)	2:32:B:ALA:HB2	2:31:B:PRO:HD3	10	1.15
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG12	3	1.15
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	13	1.15
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	2	1.15
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	6	1.15
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	6	1.15
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	8	1.15
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	8	1.15
(1,1477)	1:1644:A:LEU:HD23	1:1528:A:ASP:H	20	1.15
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG12	4	1.15
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG11	9	1.15
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	14	1.15
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	3	1.15
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	3	1.15
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	4	1.15
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	11	1.15
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	3	1.15
(1,275)	2:13:B:LEU:HD21	2:8:B:LEU:HA	2	1.15
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD3	7	1.15
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG12	7	1.15
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG11	14	1.15
(1,87)	1:1584:A:VAL:HG13	1:1585:A:ASP:HB2	10	1.15
(1,87)	1:1587:A:VAL:HG11	1:1612:A:PHE:HB3	13	1.15
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	9	1.14
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD1	14	1.14
(1,2508)	2:14:B:VAL:HG21	2:17:B:LEU:HD13	1	1.14
(1,2508)	2:14:B:VAL:HG21	2:17:B:LEU:HD13	12	1.14
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	11	1.14
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	3	1.14
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	10	1.14
(1,2186)	1:1556:A:ASN:HD22	1:1537:A:GLY:HA2	8	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	19	1.14
(1,676)	1:1529:A:LEU:HD13	1:1529:A:LEU:HB3	14	1.14
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	1	1.14
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD13	5	1.14
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD2	10	1.14
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	18	1.14
(1,496)	1:1627:A:ILE:HG21	1:1638:A:PHE:HA	6	1.14
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	14	1.14
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HB3	20	1.14
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	19	1.14
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	6	1.14
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	12	1.14
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	3	1.14
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	14	1.14
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	18	1.14
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD2	16	1.13
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	2	1.13
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	11	1.13
(1,2507)	2:14:B:VAL:HG23	2:17:B:LEU:HD21	11	1.13
(1,2296)	2:17:B:LEU:HD23	2:28:B:PHE:HB2	6	1.13
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	8	1.13
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	4	1.13
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	7	1.13
(1,1585)	1:1550:A:MET:H	1:1539:A:THR:HG23	4	1.13
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG11	10	1.13
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	12	1.13
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	6	1.13
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	13	1.13
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	14	1.13
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB2	5	1.13
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	7	1.13
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	14	1.13
(1,98)	1:1636:A:LEU:HD23	1:1606:A:TYR:HB2	1	1.13
(1,85)	1:1584:A:VAL:HG21	1:1589:A:GLN:HB3	11	1.13
(1,10)	1:1550:A:MET:HE3	1:1549:A:TYR:HA	19	1.13
(2,1)	1:1574:A:VAL:HG22	1:1636:A:LEU:H	9	1.12
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	10	1.12
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	18	1.12
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HG3	9	1.12
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD12	9	1.12
(1,2274)	2:14:B:VAL:HG23	2:18:B:GLN:HG3	7	1.12
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	16	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	20	1.12
(1,806)	1:1584:A:VAL:HG21	1:1585:A:ASP:HB2	15	1.12
(1,694)	1:1636:A:LEU:HD11	1:1635:A:THR:HA	4	1.12
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	3	1.12
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	19	1.12
(1,448)	1:1550:A:MET:HE1	1:1550:A:MET:HG3	15	1.12
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD21	5	1.12
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	11	1.12
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD11	4	1.12
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	5	1.11
(1,3007)	2:17:B:LEU:H	2:56:B:LEU:HD11	11	1.11
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD13	10	1.11
(1,2508)	2:14:B:VAL:HG22	2:17:B:LEU:HD13	19	1.11
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	7	1.11
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	18	1.11
(1,1010)	1:1548:A:VAL:HG12	1:1542:A:TYR:HD1	16	1.11
(1,663)	1:1563:A:VAL:HG23	1:1559:A:CYS:HB2	17	1.11
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD13	4	1.11
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	14	1.11
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	3	1.11
(1,496)	1:1627:A:ILE:HG21	1:1638:A:PHE:HA	15	1.11
(1,448)	1:1550:A:MET:HE2	1:1550:A:MET:HG3	4	1.11
(1,448)	1:1550:A:MET:HE2	1:1550:A:MET:HG3	5	1.11
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD13	17	1.11
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD23	19	1.11
(1,325)	2:17:B:LEU:HD11	2:14:B:VAL:HA	14	1.11
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD2	16	1.11
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD12	9	1.11
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD21	3	1.11
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	12	1.11
(1,26)	1:1591:A:VAL:HG13	1:1593:A:LYS:HE3	16	1.11
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	7	1.11
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	10	1.11
(1,3009)	2:42:B:ILE:HG23	2:17:B:LEU:HD21	8	1.1
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD22	6	1.1
(1,2445)	2:7:B:THR:HG23	2:50:B:SER:HB3	17	1.1
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	9	1.1
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	13	1.1
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	5	1.1
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD2	16	1.1
(1,613)	1:1574:A:VAL:HG13	1:1565:A:ALA:HB1	1	1.1
(1,613)	1:1574:A:VAL:HG11	1:1565:A:ALA:HB3	13	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	6	1.1
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	1	1.1
(1,448)	1:1550:A:MET:HE1	1:1550:A:MET:HG3	20	1.1
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	11	1.1
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	6	1.1
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	8	1.09
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG22	1	1.09
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	5	1.09
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	12	1.09
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	10	1.09
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG13	19	1.09
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	16	1.09
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	12	1.09
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD1	19	1.09
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	4	1.09
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	11	1.09
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	10	1.09
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	7	1.09
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG12	17	1.09
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD12	1	1.09
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD13	3	1.09
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD23	10	1.09
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD13	19	1.09
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	18	1.09
(1,11)	1:1625:A:MET:HE2	1:1626:A:LEU:HA	16	1.09
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD22	5	1.08
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	5	1.08
(1,2322)	2:32:B:ALA:HB3	2:33:B:SER:HB3	13	1.08
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	17	1.08
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	8	1.08
(1,1477)	1:1644:A:LEU:HD21	1:1528:A:ASP:H	5	1.08
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	5	1.08
(1,1067)	1:1588:A:LEU:HD13	1:1583:A:TYR:HB3	3	1.08
(1,1066)	1:1588:A:LEU:HD13	1:1518:A:VAL:HG11	11	1.08
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	17	1.08
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG23	19	1.08
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	11	1.08
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	5	1.08
(1,448)	1:1550:A:MET:HE1	1:1550:A:MET:HG3	2	1.08
(1,431)	1:1552:A:ILE:HD11	1:1610:A:ILE:HG13	5	1.08
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	6	1.08
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD21	5	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD21	8	1.08
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD22	18	1.08
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	12	1.08
(1,10)	1:1550:A:MET:HE2	1:1549:A:TYR:HA	13	1.08
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	17	1.08
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD1	8	1.07
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	9	1.07
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	4	1.07
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HG3	15	1.07
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG22	16	1.07
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	12	1.07
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	9	1.07
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	13	1.07
(1,536)	1:1609:A:VAL:HG21	1:1607:A:LYS:HE3	16	1.07
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	16	1.07
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD13	14	1.07
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD21	16	1.07
(1,229)	2:55:B:LEU:HD12	2:56:B:LEU:H	17	1.07
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	3	1.07
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	20	1.07
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	18	1.07
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	12	1.07
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD12	16	1.07
(2,1)	1:1574:A:VAL:HG21	1:1636:A:LEU:H	19	1.06
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	7	1.06
(1,2323)	2:32:B:ALA:HB1	2:33:B:SER:HB2	12	1.06
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG21	18	1.06
(1,932)	1:1601:A:LYS:HD3	1:1604:A:LEU:HD13	3	1.06
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	6	1.06
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD1	1	1.06
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD22	12	1.06
(1,98)	1:1636:A:LEU:HD21	1:1634:A:CYS:HB3	5	1.06
(1,95)	1:1602:A:SER:HB2	1:1604:A:LEU:HD22	6	1.06
(1,89)	1:1511:A:ASN:HB2	1:1521:A:PRO:HG3	11	1.06
(1,87)	1:1584:A:VAL:HG13	1:1585:A:ASP:HB2	8	1.06
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	8	1.06
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	10	1.06
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD12	20	1.06
(2,1)	1:1574:A:VAL:HG21	1:1636:A:LEU:H	18	1.05
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	13	1.05
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	8	1.05
(1,2326)	2:32:B:ALA:HB3	2:31:B:PRO:HD3	3	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2321)	2:32:B:ALA:HB1	2:33:B:SER:HA	19	1.05
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	11	1.05
(1,1214)	1:1625:A:MET:HE3	1:1641:A:HIS:H	16	1.05
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG12	18	1.05
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	20	1.05
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	12	1.05
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD1	6	1.05
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	14	1.05
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	5	1.05
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	7	1.05
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	12	1.05
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	4	1.05
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	17	1.05
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD21	4	1.05
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD13	13	1.05
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	13	1.05
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	16	1.05
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	9	1.04
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD22	20	1.04
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	7	1.04
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	13	1.04
(1,2294)	2:17:B:LEU:HD23	2:16:B:THR:H	17	1.04
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG13	1	1.04
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	14	1.04
(1,1022)	1:1552:A:ILE:HD11	1:1550:A:MET:HB3	19	1.04
(1,505)	1:1618:A:ALA:HB3	1:1616:A:PRO:HD2	15	1.04
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	2	1.04
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	10	1.04
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	18	1.04
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	2	1.04
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	8	1.04
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG22	5	1.04
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	9	1.04
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG11	15	1.04
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	8	1.04
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	11	1.04
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	17	1.04
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	12	1.04
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	1	1.04
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	20	1.04
(1,56)	1:1563:A:VAL:HG23	1:1559:A:CYS:H	20	1.04
(1,47)	1:1518:A:VAL:HG12	1:1513:A:HIS:HB3	10	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:1540:A:ALA:HB3	1:1626:A:LEU:H	4	1.04
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	10	1.04
(1,11)	1:1625:A:MET:HE3	1:1626:A:LEU:HA	19	1.04
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	17	1.04
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	19	1.03
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	6	1.03
(1,2993)	2:17:B:LEU:H	2:17:B:LEU:HD23	17	1.03
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	4	1.03
(1,2527)	2:58:B:THR:HG23	2:59:B:TYR:HB3	15	1.03
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	14	1.03
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD3	3	1.03
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD22	19	1.03
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	8	1.03
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD21	19	1.03
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	17	1.03
(1,306)	2:52:B:ASP:H	2:55:B:LEU:HB3	15	1.03
(1,263)	2:56:B:LEU:HD22	2:53:B:LEU:HB3	2	1.03
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD23	19	1.03
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD12	20	1.03
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	9	1.03
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	3	1.03
(1,12)	1:1625:A:MET:HE1	1:1620:A:PRO:HD2	11	1.03
(2,1)	1:1574:A:VAL:HG23	1:1636:A:LEU:H	7	1.02
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	1	1.02
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	19	1.02
(1,2450)	2:55:B:LEU:HD13	2:58:B:THR:HG21	2	1.02
(1,2292)	2:17:B:LEU:HD13	2:20:B:VAL:HG12	11	1.02
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	6	1.02
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	16	1.02
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	6	1.02
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD22	2	1.02
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	12	1.02
(1,505)	1:1618:A:ALA:HB3	1:1616:A:PRO:HD2	14	1.02
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	20	1.02
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	6	1.02
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	2	1.02
(1,406)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	10	1.02
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	2	1.02
(1,395)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	10	1.02
(1,372)	1:1569:A:GLN:HG3	2:15:B:ASP:HB3	19	1.02
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	6	1.02
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	8	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:1587:A:VAL:HG21	1:1586:A:GLN:HE21	13	1.02
(1,3010)	2:17:B:LEU:HD23	2:56:B:LEU:HD12	7	1.01
(1,3002)	2:42:B:ILE:HD12	2:28:B:PHE:HE1	18	1.01
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	18	1.01
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG11	6	1.01
(1,2292)	2:17:B:LEU:HD13	2:42:B:ILE:HG13	16	1.01
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	4	1.01
(1,1214)	1:1625:A:MET:HE1	1:1641:A:HIS:H	1	1.01
(1,1214)	1:1625:A:MET:HE3	1:1641:A:HIS:H	4	1.01
(1,889)	1:1544:A:LYS:HA	1:1544:A:LYS:HD2	18	1.01
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG21	4	1.01
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG21	8	1.01
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	10	1.01
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	19	1.01
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD11	9	1.01
(1,586)	1:1548:A:VAL:HG22	1:1638:A:PHE:HD1	9	1.01
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	3	1.01
(1,367)	1:1601:A:LYS:HE3	1:1604:A:LEU:H	10	1.01
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD12	17	1.01
(1,325)	2:17:B:LEU:HD12	2:28:B:PHE:HB2	4	1.01
(1,323)	2:60:B:CYS:H	2:56:B:LEU:HD22	11	1.01
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD2	16	1.01
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	9	1.01
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	14	1.01
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD11	12	1.01
(1,11)	1:1625:A:MET:HE2	1:1626:A:LEU:HA	5	1.01
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE1	15	1.0
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG11	5	1.0
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	2	1.0
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	14	1.0
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD12	15	1.0
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD21	20	1.0
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD2	1	1.0
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD2	15	1.0
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD22	11	1.0
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD12	9	1.0
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	20	1.0
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD13	2	1.0
(1,145)	1:1632:A:GLN:HB2	1:1630:A:ASP:HB3	8	1.0
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	13	1.0
(1,59)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	20	1.0
(1,49)	1:1540:A:ALA:HB1	1:1625:A:MET:HG2	11	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:1518:A:VAL:HG13	1:1513:A:HIS:HB3	9	1.0
(1,47)	1:1518:A:VAL:HG12	1:1513:A:HIS:HB2	11	1.0
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD11	12	1.0
(2,1)	1:1574:A:VAL:HG23	1:1636:A:LEU:H	16	0.99
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	9	0.99
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD23	2	0.99
(1,2714)	2:52:B:ASP:H	2:51:B:CYS:HB3	14	0.99
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	13	0.99
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	3	0.99
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	10	0.99
(1,1214)	1:1625:A:MET:HE3	1:1641:A:HIS:H	5	0.99
(1,1214)	1:1625:A:MET:HE1	1:1641:A:HIS:H	19	0.99
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	4	0.99
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	2	0.99
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	10	0.99
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	18	0.99
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	1	0.99
(1,806)	1:1584:A:VAL:HG21	1:1585:A:ASP:HB2	4	0.99
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	14	0.99
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG23	16	0.99
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	1	0.99
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD1	3	0.99
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	9	0.99
(1,496)	1:1627:A:ILE:HG21	1:1638:A:PHE:HA	13	0.99
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	17	0.99
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	18	0.99
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	18	0.99
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD12	1	0.99
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD13	3	0.99
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	14	0.99
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD13	6	0.99
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	2	0.99
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	10	0.99
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	16	0.99
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD13	5	0.99
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	1	0.98
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	14	0.98
(1,2212)	1:1606:A:TYR:H	1:1574:A:VAL:HG23	11	0.98
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD23	10	0.98
(1,994)	1:1610:A:ILE:HD12	1:1608:A:SER:HB3	4	0.98
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	7	0.98
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	13	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	18	0.98
(1,586)	1:1548:A:VAL:HG22	1:1638:A:PHE:HD1	2	0.98
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	10	0.98
(1,586)	1:1548:A:VAL:HG23	1:1638:A:PHE:HD1	19	0.98
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	13	0.98
(1,496)	1:1627:A:ILE:HG22	1:1638:A:PHE:HA	8	0.98
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	1	0.98
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	5	0.98
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	8	0.98
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD23	10	0.98
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	12	0.98
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	12	0.98
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	14	0.98
(1,11)	1:1625:A:MET:HE2	1:1626:A:LEU:HA	4	0.98
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD13	19	0.98
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	2	0.97
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	10	0.97
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD13	10	0.97
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	9	0.97
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE1	9	0.97
(1,2450)	2:55:B:LEU:HD11	2:58:B:THR:HG23	6	0.97
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	5	0.97
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	17	0.97
(1,1587)	1:1604:A:LEU:H	1:1604:A:LEU:HB2	2	0.97
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	14	0.97
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	14	0.97
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	17	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	2	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG21	6	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	12	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	14	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG21	15	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	17	0.97
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	19	0.97
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	15	0.97
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	9	0.97
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	5	0.97
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD2	14	0.97
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	13	0.97
(1,535)	1:1584:A:VAL:HG13	1:1584:A:VAL:HA	11	0.97
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD13	14	0.97
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	16	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD22	18	0.97
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	5	0.97
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD11	6	0.97
(1,173)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	1	0.97
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	11	0.97
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	1	0.97
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE2	16	0.97
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	15	0.97
(2,1)	1:1574:A:VAL:HG21	1:1636:A:LEU:H	13	0.96
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD11	8	0.96
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD1	6	0.96
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	7	0.96
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	20	0.96
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	2	0.96
(1,1961)	1:1587:A:VAL:HG12	1:1586:A:GLN:H	8	0.96
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	12	0.96
(1,1961)	1:1587:A:VAL:HG12	1:1586:A:GLN:H	13	0.96
(1,1214)	1:1625:A:MET:HE1	1:1641:A:HIS:H	18	0.96
(1,1100)	1:1626:A:LEU:HD23	1:1638:A:PHE:HA	18	0.96
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	1	0.96
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	2	0.96
(1,655)	1:1581:A:LEU:HD12	1:1588:A:LEU:HA	1	0.96
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	3	0.96
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG23	12	0.96
(1,367)	1:1601:A:LYS:HE3	1:1604:A:LEU:H	11	0.96
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	11	0.96
(1,263)	2:56:B:LEU:HD22	2:53:B:LEU:HB3	6	0.96
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	3	0.96
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	4	0.96
(1,22)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	5	0.96
(1,3002)	2:42:B:ILE:HD12	2:28:B:PHE:HE2	17	0.95
(1,2860)	2:17:B:LEU:HD11	2:28:B:PHE:HE1	17	0.95
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD2	19	0.95
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	4	0.95
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	9	0.95
(1,2321)	2:32:B:ALA:HB2	2:33:B:SER:HA	20	0.95
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	1	0.95
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	4	0.95
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	6	0.95
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	15	0.95
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	17	0.95
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	20	0.95
(1,1022)	1:1552:A:ILE:HD13	1:1550:A:MET:HB3	13	0.95
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG22	9	0.95
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD13	20	0.95
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	3	0.95
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	7	0.95
(1,536)	1:1609:A:VAL:HG22	1:1607:A:LYS:HE3	6	0.95
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	5	0.95
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	18	0.95
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	7	0.95
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	4	0.95
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD22	12	0.95
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD13	13	0.95
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD23	6	0.95
(1,98)	1:1636:A:LEU:HD21	1:1606:A:TYR:HB2	18	0.95
(1,70)	1:1550:A:MET:HG3	1:1548:A:VAL:HG23	5	0.95
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	18	0.95
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	1	0.95
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	13	0.94
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	18	0.94
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	10	0.94
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	7	0.94
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	9	0.94
(1,1961)	1:1587:A:VAL:HG12	1:1586:A:GLN:H	11	0.94
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	18	0.94
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD21	5	0.94
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD13	7	0.94
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD11	10	0.94
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	18	0.94
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	10	0.94
(1,448)	1:1550:A:MET:HE1	1:1550:A:MET:HG3	6	0.94
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	1	0.94
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	11	0.94
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	1	0.94
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	11	0.94
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	20	0.94
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	12	0.94
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	1	0.94
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	13	0.94
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	5	0.94
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	1	0.94
(1,3002)	2:42:B:ILE:HD11	2:28:B:PHE:HE2	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3002)	2:42:B:ILE:HD11	2:28:B:PHE:HE2	20	0.93
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE2	2	0.93
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	1	0.93
(1,2294)	2:17:B:LEU:HD22	2:16:B:THR:H	20	0.93
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	18	0.93
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	19	0.93
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	9	0.93
(1,1214)	1:1625:A:MET:HE1	1:1641:A:HIS:H	11	0.93
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	11	0.93
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	9	0.93
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	14	0.93
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD2	10	0.93
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	4	0.93
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD1	7	0.93
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	18	0.93
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	15	0.93
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	15	0.93
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD21	8	0.93
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD12	20	0.93
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD21	16	0.93
(1,287)	2:64:B:ALA:HA	2:63:B:PRO:HB3	19	0.93
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD1	13	0.93
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HB3	13	0.93
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	13	0.93
(1,226)	2:17:B:LEU:HD12	2:57:B:GLU:HA	17	0.93
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	15	0.93
(1,189)	1:1635:A:THR:H	1:1633:A:THR:HG23	5	0.93
(1,89)	1:1511:A:ASN:HB2	1:1521:A:PRO:HG3	17	0.93
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE1	15	0.93
(1,22)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	3	0.93
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD13	14	0.92
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	12	0.92
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	3	0.92
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	20	0.92
(1,2507)	2:14:B:VAL:HG21	2:17:B:LEU:HD22	7	0.92
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	5	0.92
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	12	0.92
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	19	0.92
(1,2292)	2:17:B:LEU:HD13	2:20:B:VAL:HG11	14	0.92
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	9	0.92
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	10	0.92
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	1	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	14	0.92
(1,1793)	1:1578:A:ASN:H	1:1578:A:ASN:HD21	9	0.92
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	18	0.92
(1,1033)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	5	0.92
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	3	0.92
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	12	0.92
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD11	1	0.92
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	8	0.92
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	2	0.92
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	10	0.92
(1,535)	1:1584:A:VAL:HG13	1:1584:A:VAL:HA	3	0.92
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD12	12	0.92
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	14	0.92
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD23	19	0.92
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG13	2	0.92
(1,284)	2:35:B:VAL:HA	2:34:B:ARG:HG2	10	0.92
(1,81)	1:1512:A:GLU:HG2	1:1515:A:ASP:H	20	0.92
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	14	0.92
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	19	0.92
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	8	0.91
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD21	2	0.91
(1,2845)	2:17:B:LEU:HD21	2:26:B:PHE:HD2	1	0.91
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	19	0.91
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG11	19	0.91
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	3	0.91
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	14	0.91
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	9	0.91
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	19	0.91
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	12	0.91
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD11	1	0.91
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	15	0.91
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	5	0.91
(1,428)	1:1552:A:ILE:HD13	1:1550:A:MET:HG3	6	0.91
(1,402)	1:1629:A:LEU:HB3	2:19:B:PHE:HE2	4	0.91
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	9	0.91
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	10	0.91
(1,271)	2:54:B:ALA:HB2	2:53:B:LEU:HD11	3	0.91
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD3	5	0.91
(1,84)	1:1512:A:GLU:HG2	1:1582:A:ARG:HD2	1	0.91
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	1	0.91
(1,3011)	2:13:B:LEU:HB3	2:13:B:LEU:H	5	0.9
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD23	2	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD2	6	0.9
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG21	8	0.9
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	2	0.9
(1,1961)	1:1587:A:VAL:HG12	1:1586:A:GLN:H	16	0.9
(1,1961)	1:1587:A:VAL:HG11	1:1586:A:GLN:H	20	0.9
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	3	0.9
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	10	0.9
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	11	0.9
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	12	0.9
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	16	0.9
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	19	0.9
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	16	0.9
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	10	0.9
(1,694)	1:1636:A:LEU:HD11	1:1635:A:THR:HA	5	0.9
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG21	4	0.9
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	1	0.9
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	7	0.9
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD2	13	0.9
(1,451)	1:1550:A:MET:HE1	1:1610:A:ILE:HG13	15	0.9
(1,423)	1:1627:A:ILE:HD11	1:1637:A:PHE:HB3	4	0.9
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG23	1	0.9
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD13	2	0.9
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD21	7	0.9
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	17	0.9
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	3	0.9
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD22	11	0.9
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	1	0.9
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	19	0.9
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	8	0.9
(1,26)	1:1591:A:VAL:HG13	1:1593:A:LYS:HE3	1	0.9
(1,5)	1:1552:A:ILE:HD12	1:1529:A:LEU:HD11	18	0.9
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD11	13	0.89
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	3	0.89
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	12	0.89
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	16	0.89
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	19	0.89
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD13	8	0.89
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	9	0.89
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	19	0.89
(1,2182)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB3	12	0.89
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	2	0.89
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	5	0.89
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	9	0.89
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	13	0.89
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	15	0.89
(1,1800)	1:1511:A:ASN:HB3	1:1511:A:ASN:HD22	17	0.89
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	1	0.89
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	13	0.89
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	1	0.89
(1,1458)	1:1544:A:LYS:HB2	1:1544:A:LYS:H	13	0.89
(1,1067)	1:1588:A:LEU:HD13	1:1583:A:TYR:HB3	4	0.89
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	10	0.89
(1,1022)	1:1552:A:ILE:HD11	1:1550:A:MET:HB3	17	0.89
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	8	0.89
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	19	0.89
(1,683)	1:1532:A:LEU:HD12	1:1644:A:LEU:HD13	19	0.89
(1,679)	1:1529:A:LEU:HD22	1:1581:A:LEU:HD13	14	0.89
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	5	0.89
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	12	0.89
(1,535)	1:1584:A:VAL:HG12	1:1584:A:VAL:HA	5	0.89
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD2	8	0.89
(1,529)	1:1584:A:VAL:HG11	1:1583:A:TYR:HD2	20	0.89
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	1	0.89
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	17	0.89
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD2	11	0.89
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	13	0.89
(1,275)	2:13:B:LEU:HD22	2:8:B:LEU:HA	12	0.89
(1,264)	2:37:B:ARG:H	2:35:B:VAL:HG13	4	0.89
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	16	0.89
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	20	0.89
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	2	0.89
(1,14)	1:1552:A:ILE:HG22	1:1529:A:LEU:HD11	4	0.89
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD12	16	0.89
(1,3009)	2:56:B:LEU:HD21	2:17:B:LEU:HD21	6	0.88
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD21	9	0.88
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	8	0.88
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	2	0.88
(1,2292)	2:17:B:LEU:HD12	2:42:B:ILE:HG13	4	0.88
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	16	0.88
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	12	0.88
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	11	0.88
(1,1587)	1:1604:A:LEU:H	1:1604:A:LEU:HB2	6	0.88
(1,1089)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	19	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:1588:A:LEU:HD13	1:1583:A:TYR:HB3	12	0.88
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG11	2	0.88
(1,1054)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	16	0.88
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	7	0.88
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	1	0.88
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	13	0.88
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD2	10	0.88
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD13	5	0.88
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD21	3	0.88
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	3	0.88
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	5	0.88
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	9	0.88
(1,229)	2:55:B:LEU:HD12	2:56:B:LEU:H	7	0.88
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD21	1	0.88
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	20	0.88
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	11	0.88
(1,125)	1:1591:A:VAL:HG22	1:1592:A:TYR:HB3	15	0.88
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	3	0.88
(1,62)	1:1588:A:LEU:HD12	1:1645:A:ALA:HA	3	0.88
(1,40)	1:1587:A:VAL:HG22	1:1586:A:GLN:HE21	3	0.88
(1,3006)	2:56:B:LEU:HD13	2:42:B:ILE:HD13	20	0.87
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	15	0.87
(1,2451)	2:62:B:THR:HG22	2:63:B:PRO:HB3	20	0.87
(1,2321)	2:32:B:ALA:HB2	2:36:B:SER:HA	6	0.87
(1,2259)	2:42:B:ILE:HG23	2:28:B:PHE:HD1	10	0.87
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	7	0.87
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	3	0.87
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	8	0.87
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	20	0.87
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	18	0.87
(1,1620)	1:1558:A:ASN:H	1:1557:A:GLU:HG2	2	0.87
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	14	0.87
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	19	0.87
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	7	0.87
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	12	0.87
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	14	0.87
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	9	0.87
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	16	0.87
(1,876)	1:1585:A:ASP:HA	1:1584:A:VAL:HG23	16	0.87
(1,806)	1:1584:A:VAL:HG22	1:1585:A:ASP:HB2	7	0.87
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD2	1	0.87
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	8	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	4	0.87
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD1	16	0.87
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	12	0.87
(1,496)	1:1627:A:ILE:HG23	1:1638:A:PHE:HA	17	0.87
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	20	0.87
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD2	20	0.87
(1,388)	2:23:B:ASP:HB3	2:22:B:GLY:H	16	0.87
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	10	0.87
(1,263)	2:56:B:LEU:HD22	2:53:B:LEU:HB3	5	0.87
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG3	13	0.87
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	17	0.87
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	7	0.87
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	14	0.87
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	19	0.87
(1,98)	1:1636:A:LEU:HD21	1:1606:A:TYR:HB2	14	0.87
(1,89)	1:1511:A:ASN:HB2	1:1508:A:MET:HE1	9	0.87
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	11	0.87
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	14	0.87
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	5	0.87
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD11	2	0.87
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	9	0.87
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	1	0.86
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	11	0.86
(1,2445)	2:7:B:THR:HG23	2:50:B:SER:HB3	20	0.86
(1,2339)	2:18:B:GLN:HG3	2:26:B:PHE:HD2	3	0.86
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG11	2	0.86
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	12	0.86
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	13	0.86
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG2	2	0.86
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	5	0.86
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	2	0.86
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	2	0.86
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	4	0.86
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	7	0.86
(1,642)	1:1518:A:VAL:HG12	1:1518:A:VAL:HA	5	0.86
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD11	17	0.86
(1,610)	1:1626:A:LEU:HD13	1:1637:A:PHE:HB2	18	0.86
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD11	6	0.86
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	13	0.86
(1,325)	2:17:B:LEU:HD11	2:14:B:VAL:HA	11	0.86
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	14	0.86
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB1	18	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	20	0.86
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	14	0.86
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	14	0.86
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	15	0.86
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	11	0.86
(1,42)	1:1548:A:VAL:HG12	1:1542:A:TYR:HD1	16	0.86
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	18	0.85
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	19	0.85
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD11	17	0.85
(1,2283)	2:42:B:ILE:HD12	2:43:B:VAL:H	4	0.85
(1,2283)	2:42:B:ILE:HD12	2:43:B:VAL:H	7	0.85
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA2	6	0.85
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	10	0.85
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	13	0.85
(1,2067)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	5	0.85
(1,1800)	1:1511:A:ASN:HB2	1:1511:A:ASN:HD22	18	0.85
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	13	0.85
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	6	0.85
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	10	0.85
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	13	0.85
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	18	0.85
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	19	0.85
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	20	0.85
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	7	0.85
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	11	0.85
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	19	0.85
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG21	16	0.85
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	20	0.85
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	10	0.85
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	8	0.85
(1,642)	1:1518:A:VAL:HG11	1:1518:A:VAL:HA	12	0.85
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	8	0.85
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	15	0.85
(1,497)	1:1645:A:ALA:HB3	1:1529:A:LEU:HD11	13	0.85
(1,379)	1:1632:A:GLN:HG3	2:53:B:LEU:HD23	9	0.85
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	5	0.85
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	5	0.85
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	4	0.85
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	8	0.85
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	5	0.85
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	15	0.85
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	16	0.84
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	5	0.84
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	2	0.84
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	10	0.84
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	12	0.84
(1,2315)	2:43:B:VAL:HG23	2:40:B:ARG:HD2	6	0.84
(1,2289)	2:42:B:ILE:HD12	2:55:B:LEU:HD13	10	0.84
(1,1961)	1:1587:A:VAL:HG13	1:1586:A:GLN:H	5	0.84
(1,1858)	1:1602:A:SER:HB2	1:1602:A:SER:H	11	0.84
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG12	5	0.84
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD12	8	0.84
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	13	0.84
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	6	0.84
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	20	0.84
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	4	0.84
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	9	0.84
(1,1191)	1:1627:A:ILE:H	1:1626:A:LEU:HD12	18	0.84
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	5	0.84
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	11	0.84
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	15	0.84
(1,1033)	1:1645:A:ALA:HB1	1:1614:A:CYS:HB3	10	0.84
(1,1033)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	20	0.84
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	17	0.84
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	7	0.84
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	7	0.84
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	15	0.84
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD1	17	0.84
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE2	10	0.84
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	14	0.84
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG3	13	0.84
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG12	14	0.84
(1,369)	2:16:B:THR:H	1:1570:A:THR:HG22	16	0.84
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	3	0.84
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	4	0.84
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	2	0.84
(1,98)	1:1636:A:LEU:HD21	1:1606:A:TYR:HB2	19	0.84
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	2	0.84
(1,25)	1:1584:A:VAL:HG12	1:1582:A:ARG:HD3	8	0.84
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	2	0.84
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG12	3	0.83
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	15	0.83
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD12	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2860)	2:17:B:LEU:HD11	2:28:B:PHE:HE2	3	0.83
(1,2845)	2:17:B:LEU:HD22	2:26:B:PHE:HD1	13	0.83
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	16	0.83
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	2	0.83
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	17	0.83
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	7	0.83
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	4	0.83
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	13	0.83
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	13	0.83
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	16	0.83
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	11	0.83
(1,1587)	1:1604:A:LEU:H	1:1604:A:LEU:HB2	13	0.83
(1,1396)	1:1591:A:VAL:HG12	1:1591:A:VAL:H	18	0.83
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	13	0.83
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	8	0.83
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	9	0.83
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	19	0.83
(1,1066)	1:1588:A:LEU:HD12	1:1518:A:VAL:HG11	13	0.83
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD13	4	0.83
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	4	0.83
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	13	0.83
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	18	0.83
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	13	0.83
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG21	15	0.83
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD13	4	0.83
(1,609)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	16	0.83
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	13	0.83
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD2	16	0.83
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	19	0.83
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	10	0.83
(1,388)	2:23:B:ASP:HB3	2:22:B:GLY:H	3	0.83
(1,372)	1:1569:A:GLN:HG2	2:15:B:ASP:HB3	14	0.83
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	9	0.83
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	16	0.83
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	17	0.83
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	10	0.83
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	10	0.83
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	12	0.83
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	3	0.83
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	15	0.83
(1,147)	1:1638:A:PHE:HD1	1:1610:A:ILE:HD13	14	0.83
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD21	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	4	0.83
(1,66)	1:1636:A:LEU:HD13	1:1638:A:PHE:HZ	18	0.83
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	3	0.83
(1,40)	1:1587:A:VAL:HG23	1:1586:A:GLN:HE21	12	0.83
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	10	0.83
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	6	0.82
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	4	0.82
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	18	0.82
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	7	0.82
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	5	0.82
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	6	0.82
(1,2482)	2:13:B:LEU:HD13	2:12:B:GLU:HB3	3	0.82
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	2	0.82
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	11	0.82
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	7	0.82
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	17	0.82
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	18	0.82
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	20	0.82
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	15	0.82
(1,1858)	1:1602:A:SER:HB2	1:1602:A:SER:H	12	0.82
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	7	0.82
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	20	0.82
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	16	0.82
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	17	0.82
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	2	0.82
(1,1066)	1:1588:A:LEU:HD11	1:1518:A:VAL:HG11	1	0.82
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	14	0.82
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	1	0.82
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	1	0.82
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	15	0.82
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	11	0.82
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG23	8	0.82
(1,710)	1:1629:A:LEU:HD11	1:1629:A:LEU:H	5	0.82
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	2	0.82
(1,619)	1:1626:A:LEU:HD23	1:1629:A:LEU:HD12	3	0.82
(1,617)	1:1529:A:LEU:HD22	1:1581:A:LEU:HD13	14	0.82
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	14	0.82
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	11	0.82
(1,536)	1:1609:A:VAL:HG21	1:1607:A:LYS:HE3	19	0.82
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE1	8	0.82
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	16	0.82
(1,406)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	8	0.82
(1,387)	1:1572:A:ILE:HD11	2:16:B:THR:H	12	0.82
(1,372)	1:1569:A:GLN:HG2	2:15:B:ASP:HB3	18	0.82
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	17	0.82
(1,267)	2:35:B:VAL:HG23	2:34:B:ARG:HD3	8	0.82
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	7	0.82
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	2	0.82
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	4	0.82
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG12	20	0.82
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	18	0.82
(1,89)	1:1511:A:ASN:HB2	1:1508:A:MET:HE1	7	0.82
(1,87)	1:1584:A:VAL:HG11	1:1585:A:ASP:HB2	5	0.82
(1,79)	1:1632:A:GLN:HG3	1:1631:A:LYS:H	5	0.82
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	16	0.82
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	20	0.82
(1,25)	1:1584:A:VAL:HG13	1:1582:A:ARG:HD3	17	0.82
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG13	2	0.81
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	18	0.81
(1,2507)	2:14:B:VAL:HG23	2:17:B:LEU:HD23	2	0.81
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE1	6	0.81
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	17	0.81
(1,2274)	2:14:B:VAL:HG22	2:18:B:GLN:HG3	11	0.81
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	7	0.81
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	8	0.81
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	18	0.81
(1,1858)	1:1602:A:SER:HB2	1:1602:A:SER:H	15	0.81
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	7	0.81
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	14	0.81
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	7	0.81
(1,1179)	1:1610:A:ILE:H	1:1610:A:ILE:HG13	3	0.81
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	1	0.81
(1,1022)	1:1552:A:ILE:HD11	1:1550:A:MET:HB3	18	0.81
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	18	0.81
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	14	0.81
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG21	20	0.81
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	4	0.81
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	1	0.81
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	18	0.81
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD12	2	0.81
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	6	0.81
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD11	11	0.81
(1,586)	1:1548:A:VAL:HG23	1:1638:A:PHE:HD1	20	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	5	0.81
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	11	0.81
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	9	0.81
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	9	0.81
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD23	19	0.81
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	12	0.81
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	14	0.81
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	20	0.81
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	7	0.81
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	13	0.81
(1,199)	1:1555:A:GLU:H	1:1564:A:GLY:HA3	20	0.81
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	19	0.81
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	13	0.81
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	13	0.81
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	17	0.81
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	20	0.81
(1,124)	1:1613:A:VAL:HG21	1:1611:A:SER:HB2	3	0.81
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	20	0.81
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	2	0.81
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	15	0.81
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	15	0.8
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG13	16	0.8
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	14	0.8
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	11	0.8
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	8	0.8
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	12	0.8
(1,2322)	2:32:B:ALA:HB3	2:33:B:SER:HB3	4	0.8
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	13	0.8
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	19	0.8
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	14	0.8
(1,1022)	1:1552:A:ILE:HD13	1:1550:A:MET:HB3	6	0.8
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD23	6	0.8
(1,1003)	1:1644:A:LEU:HD22	1:1532:A:LEU:H	18	0.8
(1,904)	1:1601:A:LYS:HG2	1:1602:A:SER:HB2	19	0.8
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	1	0.8
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	4	0.8
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	14	0.8
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	10	0.8
(1,710)	1:1629:A:LEU:HD23	1:1629:A:LEU:H	9	0.8
(1,710)	1:1629:A:LEU:HD11	1:1629:A:LEU:H	10	0.8
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	15	0.8
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD11	11	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	15	0.8
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD13	16	0.8
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG21	11	0.8
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	6	0.8
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	12	0.8
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	20	0.8
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD2	8	0.8
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	9	0.8
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE2	9	0.8
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	14	0.8
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	14	0.8
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD22	11	0.8
(1,325)	2:17:B:LEU:HD11	2:28:B:PHE:HB2	2	0.8
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	6	0.8
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	10	0.8
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	18	0.8
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	9	0.8
(1,98)	1:1636:A:LEU:HD22	1:1634:A:CYS:HB3	4	0.8
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	2	0.8
(1,59)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	15	0.8
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	16	0.8
(1,49)	1:1540:A:ALA:HB1	1:1625:A:MET:HG2	15	0.8
(1,39)	1:1548:A:VAL:HG23	1:1542:A:TYR:HE2	20	0.8
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	12	0.79
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	17	0.79
(1,2868)	2:17:B:LEU:HD11	2:28:B:PHE:HD1	17	0.79
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	10	0.79
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	9	0.79
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	6	0.79
(1,2292)	2:17:B:LEU:HD12	2:20:B:VAL:HG12	12	0.79
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	2	0.79
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	9	0.79
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	14	0.79
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	11	0.79
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	16	0.79
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	12	0.79
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	10	0.79
(1,710)	1:1629:A:LEU:HD11	1:1629:A:LEU:H	8	0.79
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	19	0.79
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	2	0.79
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	3	0.79
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	19	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD11	14	0.79
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	11	0.79
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	18	0.79
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	10	0.79
(1,125)	1:1591:A:VAL:HG22	1:1592:A:TYR:HB3	6	0.79
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	6	0.79
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	15	0.79
(1,70)	1:1550:A:MET:HG3	1:1548:A:VAL:HG21	15	0.79
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	6	0.79
(1,56)	1:1563:A:VAL:HG22	1:1572:A:ILE:H	15	0.79
(1,3011)	2:13:B:LEU:HB3	2:13:B:LEU:H	16	0.78
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE1	7	0.78
(1,2860)	2:17:B:LEU:HD11	2:28:B:PHE:HE1	13	0.78
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD22	12	0.78
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	18	0.78
(1,2670)	2:21:B:CYS:H	2:20:B:VAL:HG11	4	0.78
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	19	0.78
(1,2321)	2:32:B:ALA:HB3	2:36:B:SER:HA	18	0.78
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	9	0.78
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	19	0.78
(1,2232)	1:1567:A:PHE:HD2	1:1606:A:TYR:HE2	1	0.78
(1,2232)	1:1567:A:PHE:HD2	1:1542:A:TYR:HE2	4	0.78
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	3	0.78
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	20	0.78
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	19	0.78
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	14	0.78
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	14	0.78
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	2	0.78
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	13	0.78
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	20	0.78
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	7	0.78
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	10	0.78
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG21	6	0.78
(1,710)	1:1629:A:LEU:HD12	1:1629:A:LEU:H	11	0.78
(1,710)	1:1629:A:LEU:HD13	1:1629:A:LEU:H	14	0.78
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	20	0.78
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	9	0.78
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	14	0.78
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD23	16	0.78
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	11	0.78
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	6	0.78
(1,584)	1:1540:A:ALA:HB3	1:1638:A:PHE:HD2	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG23	2	0.78
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG22	14	0.78
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	19	0.78
(1,440)	1:1550:A:MET:HE3	1:1638:A:PHE:HD1	9	0.78
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	10	0.78
(1,399)	2:19:B:PHE:HD2	2:16:B:THR:HG22	18	0.78
(1,388)	2:23:B:ASP:HB3	2:22:B:GLY:H	19	0.78
(1,325)	2:17:B:LEU:HD12	2:14:B:VAL:HA	7	0.78
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	20	0.78
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	1	0.78
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	1	0.78
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	17	0.78
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	16	0.78
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	9	0.78
(1,227)	2:17:B:LEU:HD21	2:26:B:PHE:HB2	11	0.78
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	18	0.78
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	6	0.78
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	16	0.78
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	8	0.78
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	6	0.78
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	19	0.78
(1,22)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	11	0.78
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	6	0.77
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	11	0.77
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD23	15	0.77
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD1	2	0.77
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD22	16	0.77
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	13	0.77
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	18	0.77
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD22	19	0.77
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG21	6	0.77
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE2	5	0.77
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	6	0.77
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	8	0.77
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	3	0.77
(1,2292)	2:17:B:LEU:HD11	2:20:B:VAL:HG11	15	0.77
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD13	16	0.77
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	12	0.77
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	1	0.77
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	9	0.77
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	1	0.77
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	13	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	17	0.77
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	5	0.77
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	16	0.77
(1,1031)	1:1577:A:ALA:HB3	1:1562:A:GLY:HA3	1	0.77
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	16	0.77
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	5	0.77
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE1	14	0.77
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	3	0.77
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	14	0.77
(1,710)	1:1629:A:LEU:HD13	1:1629:A:LEU:H	15	0.77
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	18	0.77
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD1	12	0.77
(1,683)	1:1532:A:LEU:HD11	1:1644:A:LEU:HD13	11	0.77
(1,677)	1:1529:A:LEU:HD12	1:1590:A:LEU:HD11	7	0.77
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	11	0.77
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	20	0.77
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD21	3	0.77
(1,636)	1:1588:A:LEU:HD22	1:1529:A:LEU:HD12	12	0.77
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	19	0.77
(1,597)	1:1529:A:LEU:HD21	1:1529:A:LEU:HA	14	0.77
(1,587)	1:1548:A:VAL:HG12	1:1542:A:TYR:HE2	20	0.77
(1,584)	1:1540:A:ALA:HB3	1:1638:A:PHE:HD2	11	0.77
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	15	0.77
(1,524)	1:1577:A:ALA:HB1	1:1592:A:TYR:HE2	20	0.77
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	7	0.77
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD13	13	0.77
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD2	7	0.77
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	8	0.77
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	20	0.77
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD12	16	0.77
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	4	0.77
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	2	0.77
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	16	0.77
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	4	0.77
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	10	0.77
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	18	0.77
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG21	6	0.77
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	3	0.77
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	7	0.77
(1,32)	1:1547:A:VAL:HG23	1:1549:A:TYR:HB3	7	0.77
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	1	0.77
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2992)	2:42:B:ILE:HD11	2:59:B:TYR:HE2	15	0.76
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	13	0.76
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	3	0.76
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	13	0.76
(1,2441)	2:8:B:LEU:HD11	2:8:B:LEU:HA	8	0.76
(1,2284)	2:42:B:ILE:HD12	2:42:B:ILE:H	10	0.76
(1,2232)	1:1567:A:PHE:HD2	1:1606:A:TYR:HE2	3	0.76
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG13	5	0.76
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD13	5	0.76
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG23	4	0.76
(1,686)	1:1644:A:LEU:HD21	1:1529:A:LEU:HA	20	0.76
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	12	0.76
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD21	10	0.76
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD12	4	0.76
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG21	19	0.76
(1,524)	1:1577:A:ALA:HB1	1:1592:A:TYR:HE1	2	0.76
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	16	0.76
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	3	0.76
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	6	0.76
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	7	0.76
(1,372)	1:1569:A:GLN:HG3	2:15:B:ASP:HB3	20	0.76
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD2	14	0.76
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	1	0.76
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	8	0.76
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	8	0.76
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	17	0.76
(1,227)	2:17:B:LEU:HD23	2:26:B:PHE:HB2	18	0.76
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	10	0.76
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	16	0.76
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	15	0.76
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	17	0.76
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	19	0.76
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	13	0.76
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	15	0.76
(1,116)	1:1613:A:VAL:HG11	1:1642:A:THR:H	12	0.76
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	5	0.76
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	15	0.76
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	4	0.76
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	9	0.76
(1,66)	1:1636:A:LEU:HD13	1:1638:A:PHE:HZ	10	0.76
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	19	0.76
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE2	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:1609:A:VAL:HG23	1:1637:A:PHE:HB3	6	0.76
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	17	0.76
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	16	0.75
(1,2874)	2:17:B:LEU:HD12	2:28:B:PHE:HD1	20	0.75
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD22	6	0.75
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	1	0.75
(1,2670)	2:21:B:CYS:H	2:20:B:VAL:HG11	9	0.75
(1,2670)	2:21:B:CYS:H	2:20:B:VAL:HG11	13	0.75
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	6	0.75
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	11	0.75
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG21	3	0.75
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	12	0.75
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD13	1	0.75
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA3	5	0.75
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	10	0.75
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	15	0.75
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	8	0.75
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	8	0.75
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	12	0.75
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	10	0.75
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	2	0.75
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	3	0.75
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	6	0.75
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	12	0.75
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	15	0.75
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	9	0.75
(1,806)	1:1584:A:VAL:HG21	1:1585:A:ASP:HB2	6	0.75
(1,790)	1:1589:A:GLN:HG3	1:1589:A:GLN:HE21	2	0.75
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG21	17	0.75
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	1	0.75
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	16	0.75
(1,710)	1:1629:A:LEU:HD22	1:1629:A:LEU:H	19	0.75
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD2	6	0.75
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	8	0.75
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD12	18	0.75
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG22	18	0.75
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	9	0.75
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD1	5	0.75
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD11	3	0.75
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD12	6	0.75
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE2	7	0.75
(1,402)	1:1629:A:LEU:HB3	2:19:B:PHE:HE2	9	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD21	16	0.75
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	9	0.75
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD11	7	0.75
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	16	0.75
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	9	0.75
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	2	0.75
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	11	0.75
(1,234)	2:55:B:LEU:HD12	2:54:B:ALA:HB3	15	0.75
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	13	0.75
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	14	0.75
(1,204)	1:1610:A:ILE:HG22	1:1639:A:SER:H	1	0.75
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	18	0.75
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG21	15	0.75
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	19	0.75
(1,89)	1:1511:A:ASN:HB2	1:1508:A:MET:HE1	8	0.75
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	2	0.75
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	13	0.75
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB1	9	0.75
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	8	0.75
(1,62)	1:1588:A:LEU:HD12	1:1645:A:ALA:HA	8	0.75
(1,56)	1:1563:A:VAL:HG23	1:1559:A:CYS:H	17	0.75
(1,5)	1:1552:A:ILE:HD13	1:1529:A:LEU:HD13	11	0.75
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD23	3	0.74
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	9	0.74
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	16	0.74
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	9	0.74
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	19	0.74
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	16	0.74
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	6	0.74
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	18	0.74
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	13	0.74
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	5	0.74
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	10	0.74
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	15	0.74
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	1	0.74
(1,1858)	1:1602:A:SER:HB2	1:1602:A:SER:H	3	0.74
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	12	0.74
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	7	0.74
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG12	11	0.74
(1,1396)	1:1591:A:VAL:HG12	1:1591:A:VAL:H	3	0.74
(1,1396)	1:1591:A:VAL:HG12	1:1591:A:VAL:H	17	0.74
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	17	0.74
(1,1201)	1:1587:A:VAL:HG21	1:1584:A:VAL:H	14	0.74
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	18	0.74
(1,1067)	1:1588:A:LEU:HD13	1:1583:A:TYR:HB3	8	0.74
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD1	18	0.74
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	17	0.74
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	18	0.74
(1,569)	1:1547:A:VAL:HG12	1:1539:A:THR:HG23	10	0.74
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD2	17	0.74
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	15	0.74
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	6	0.74
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	3	0.74
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	7	0.74
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	2	0.74
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	13	0.74
(1,287)	2:64:B:ALA:HA	2:63:B:PRO:HB3	1	0.74
(1,277)	2:56:B:LEU:HD12	2:53:B:LEU:H	5	0.74
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	12	0.74
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	9	0.74
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	1	0.74
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	9	0.74
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	14	0.74
(1,125)	1:1591:A:VAL:HG21	1:1592:A:TYR:HB3	5	0.74
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	16	0.74
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	20	0.74
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	6	0.74
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	13	0.74
(1,14)	1:1552:A:ILE:HG22	1:1529:A:LEU:HD12	7	0.74
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	19	0.74
(1,2987)	2:42:B:ILE:HD13	2:56:B:LEU:HG	6	0.73
(1,2884)	2:43:B:VAL:HG21	2:28:B:PHE:HD1	12	0.73
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	14	0.73
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	17	0.73
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	15	0.73
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD22	9	0.73
(1,2714)	2:52:B:ASP:H	2:51:B:CYS:HB3	1	0.73
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	2	0.73
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	16	0.73
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	14	0.73
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	15	0.73
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	1	0.73
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	20	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2278)	2:42:B:ILE:HD13	2:55:B:LEU:HB3	20	0.73
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	10	0.73
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	14	0.73
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	19	0.73
(1,2149)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	6	0.73
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	10	0.73
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	11	0.73
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	7	0.73
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	1	0.73
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	5	0.73
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	1	0.73
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	18	0.73
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	11	0.73
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	15	0.73
(1,806)	1:1584:A:VAL:HG21	1:1585:A:ASP:HB2	8	0.73
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	4	0.73
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	2	0.73
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	7	0.73
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	12	0.73
(1,708)	1:1590:A:LEU:HD12	1:1592:A:TYR:HD1	13	0.73
(1,660)	1:1636:A:LEU:HD13	1:1636:A:LEU:HA	5	0.73
(1,645)	1:1529:A:LEU:HD12	1:1612:A:PHE:HD1	14	0.73
(1,645)	1:1529:A:LEU:HD12	1:1612:A:PHE:HD2	14	0.73
(1,619)	1:1626:A:LEU:HD21	1:1629:A:LEU:HD12	14	0.73
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	19	0.73
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	18	0.73
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	20	0.73
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	10	0.73
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD12	1	0.73
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	14	0.73
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	16	0.73
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	16	0.73
(1,387)	1:1572:A:ILE:HD12	2:16:B:THR:H	11	0.73
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD23	7	0.73
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	4	0.73
(1,325)	2:17:B:LEU:HD11	2:28:B:PHE:HB2	1	0.73
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	13	0.73
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	4	0.73
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	5	0.73
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	14	0.73
(1,227)	2:17:B:LEU:HD22	2:26:B:PHE:HB2	7	0.73
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	5	0.73
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	16	0.73
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	17	0.73
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	7	0.73
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	20	0.73
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD21	14	0.72
(1,3006)	2:56:B:LEU:HD12	2:42:B:ILE:HD11	18	0.72
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	8	0.72
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	15	0.72
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	10	0.72
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	17	0.72
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	15	0.72
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	20	0.72
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	6	0.72
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	19	0.72
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE2	1	0.72
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	15	0.72
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	19	0.72
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	8	0.72
(1,2284)	2:42:B:ILE:HD12	2:42:B:ILE:H	14	0.72
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	9	0.72
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG13	11	0.72
(1,1992)	1:1523:A:THR:H	1:1521:A:PRO:HG3	3	0.72
(1,1849)	1:1621:A:THR:HG23	1:1621:A:THR:H	2	0.72
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	1	0.72
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	13	0.72
(1,1447)	1:1548:A:VAL:HG13	1:1548:A:VAL:H	4	0.72
(1,1396)	1:1591:A:VAL:HG13	1:1591:A:VAL:H	8	0.72
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	7	0.72
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	3	0.72
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	20	0.72
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	3	0.72
(1,1089)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	11	0.72
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	7	0.72
(1,1004)	1:1644:A:LEU:HD22	1:1645:A:ALA:H	20	0.72
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG21	2	0.72
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	10	0.72
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG21	11	0.72
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD12	8	0.72
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	11	0.72
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	11	0.72
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	19	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	11	0.72
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	19	0.72
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	16	0.72
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD2	5	0.72
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD1	8	0.72
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD21	10	0.72
(1,372)	1:1569:A:GLN:HG2	2:15:B:ASP:HB3	15	0.72
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	16	0.72
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	10	0.72
(1,266)	2:62:B:THR:HG22	2:24:B:ARG:HG3	20	0.72
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	6	0.72
(1,245)	2:42:B:ILE:HD13	2:26:B:PHE:HB2	4	0.72
(1,245)	2:42:B:ILE:HD12	2:14:B:VAL:HA	17	0.72
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	8	0.72
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	18	0.72
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	6	0.72
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	19	0.72
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	2	0.72
(1,139)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	9	0.72
(1,125)	1:1591:A:VAL:HG21	1:1592:A:TYR:HB3	1	0.72
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	7	0.72
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	19	0.72
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	15	0.72
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	17	0.72
(1,55)	1:1518:A:VAL:HG13	1:1511:A:ASN:HB2	20	0.72
(1,28)	1:1609:A:VAL:HG21	1:1607:A:LYS:HB3	20	0.72
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	8	0.72
(1,3006)	2:56:B:LEU:HD11	2:42:B:ILE:HD12	19	0.71
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	10	0.71
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	16	0.71
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB3	15	0.71
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	8	0.71
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	2	0.71
(1,2529)	2:43:B:VAL:HG22	2:44:B:GLU:HG3	19	0.71
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	13	0.71
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	1	0.71
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	2	0.71
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	7	0.71
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG12	11	0.71
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	17	0.71
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD3	8	0.71
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	7	0.71
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	16	0.71
(1,2284)	2:42:B:ILE:HD12	2:42:B:ILE:H	20	0.71
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	18	0.71
(1,2149)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	19	0.71
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	6	0.71
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	8	0.71
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	11	0.71
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	4	0.71
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	5	0.71
(1,1136)	1:1590:A:LEU:HD23	1:1554:A:GLY:H	19	0.71
(1,1063)	1:1644:A:LEU:HD13	1:1644:A:LEU:HB3	20	0.71
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	1	0.71
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	14	0.71
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	15	0.71
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	9	0.71
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG22	19	0.71
(1,710)	1:1629:A:LEU:HD23	1:1629:A:LEU:H	4	0.71
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	11	0.71
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	13	0.71
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG21	5	0.71
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	14	0.71
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	4	0.71
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD11	11	0.71
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD12	16	0.71
(1,424)	1:1552:A:ILE:HD11	1:1592:A:TYR:HH	6	0.71
(1,423)	1:1627:A:ILE:HD12	1:1637:A:PHE:HB3	1	0.71
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	4	0.71
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA2	20	0.71
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB1	14	0.71
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	14	0.71
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG3	19	0.71
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	4	0.71
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	15	0.71
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	12	0.71
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG23	6	0.71
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	17	0.71
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	3	0.71
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	3	0.71
(1,79)	1:1632:A:GLN:HG3	1:1631:A:LYS:H	9	0.71
(1,30)	1:1587:A:VAL:HG21	1:1585:A:ASP:H	14	0.71
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	4	0.71
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	13	0.71
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	4	0.7
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD21	5	0.7
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	4	0.7
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD22	1	0.7
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB1	1	0.7
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	8	0.7
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	3	0.7
(1,2499)	2:56:B:LEU:HD13	2:20:B:VAL:HB	8	0.7
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	5	0.7
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	9	0.7
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	12	0.7
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	3	0.7
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	11	0.7
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	2	0.7
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	9	0.7
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	12	0.7
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG21	15	0.7
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	18	0.7
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	12	0.7
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	4	0.7
(1,2241)	1:1527:A:PHE:HD2	1:1519:A:THR:HA	5	0.7
(1,2186)	1:1556:A:ASN:HD22	1:1537:A:GLY:HA2	20	0.7
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	4	0.7
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	8	0.7
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	2	0.7
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	1	0.7
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	18	0.7
(1,1022)	1:1552:A:ILE:HD11	1:1550:A:MET:HB3	9	0.7
(1,1022)	1:1552:A:ILE:HD13	1:1550:A:MET:HB3	12	0.7
(1,1003)	1:1644:A:LEU:HD22	1:1532:A:LEU:H	13	0.7
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	9	0.7
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	20	0.7
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	20	0.7
(1,733)	1:1582:A:ARG:HG2	1:1582:A:ARG:H	3	0.7
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	9	0.7
(1,718)	1:1581:A:LEU:HD23	1:1518:A:VAL:HG22	13	0.7
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG22	18	0.7
(1,710)	1:1629:A:LEU:HD13	1:1629:A:LEU:H	13	0.7
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	3	0.7
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	2	0.7
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	7	0.7
(1,586)	1:1548:A:VAL:HG23	1:1638:A:PHE:HD2	11	0.7
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	9	0.7
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	13	0.7
(1,536)	1:1609:A:VAL:HG23	1:1607:A:LYS:HE3	7	0.7
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD21	4	0.7
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG3	2	0.7
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	18	0.7
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG22	3	0.7
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	16	0.7
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	12	0.7
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	13	0.7
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD11	15	0.7
(1,277)	2:56:B:LEU:HD13	2:53:B:LEU:H	9	0.7
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	6	0.7
(1,248)	2:29:B:SER:HB3	2:30:B:ARG:HG2	2	0.7
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	3	0.7
(1,236)	2:20:B:VAL:HG13	2:19:B:PHE:HA	12	0.7
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	12	0.7
(1,173)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	8	0.7
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	10	0.7
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	17	0.7
(1,129)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	2	0.7
(1,79)	1:1632:A:GLN:HG2	1:1631:A:LYS:H	8	0.7
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	13	0.7
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	1	0.7
(1,32)	1:1547:A:VAL:HG23	1:1567:A:PHE:HB3	2	0.7
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	9	0.7
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	13	0.7
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	5	0.69
(2,1)	1:1636:A:LEU:H	1:1626:A:LEU:HD22	12	0.69
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	12	0.69
(1,3010)	2:17:B:LEU:HD22	2:56:B:LEU:HD11	11	0.69
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	17	0.69
(1,2869)	2:17:B:LEU:HD21	2:28:B:PHE:HD1	16	0.69
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	8	0.69
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	9	0.69
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD22	19	0.69
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB3	5	0.69
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	7	0.69
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	14	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2445)	2:7:B:THR:HG22	2:50:B:SER:HB3	11	0.69
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB2	3	0.69
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	5	0.69
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	14	0.69
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG23	7	0.69
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	3	0.69
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	4	0.69
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD21	3	0.69
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD13	16	0.69
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	10	0.69
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	17	0.69
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	15	0.69
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	16	0.69
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	8	0.69
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	9	0.69
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG12	12	0.69
(1,1063)	1:1644:A:LEU:HD11	1:1644:A:LEU:HB3	5	0.69
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	13	0.69
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	14	0.69
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	4	0.69
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	17	0.69
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	7	0.69
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG22	15	0.69
(1,718)	1:1581:A:LEU:HD21	1:1518:A:VAL:HG22	3	0.69
(1,710)	1:1629:A:LEU:HD21	1:1629:A:LEU:H	3	0.69
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	8	0.69
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	17	0.69
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	13	0.69
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	16	0.69
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	17	0.69
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD12	15	0.69
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD1	10	0.69
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE1	19	0.69
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	18	0.69
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	9	0.69
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	6	0.69
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	12	0.69
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	16	0.69
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	10	0.69
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	6	0.69
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	18	0.69
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	18	0.69
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	2	0.69
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	19	0.69
(1,124)	1:1613:A:VAL:HG23	1:1611:A:SER:HB2	5	0.69
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	19	0.69
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	17	0.69
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	5	0.69
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	3	0.69
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	7	0.69
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	5	0.69
(1,27)	1:1609:A:VAL:HG23	1:1637:A:PHE:HB3	11	0.69
(1,27)	1:1609:A:VAL:HG22	1:1637:A:PHE:HB3	18	0.69
(1,2992)	2:42:B:ILE:HD12	2:59:B:TYR:HE2	6	0.68
(1,2884)	2:43:B:VAL:HG21	2:28:B:PHE:HD2	11	0.68
(1,2884)	2:43:B:VAL:HG21	2:28:B:PHE:HD2	18	0.68
(1,2860)	2:17:B:LEU:HD13	2:28:B:PHE:HE1	18	0.68
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	9	0.68
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	4	0.68
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	5	0.68
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	17	0.68
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	20	0.68
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	10	0.68
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	18	0.68
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	15	0.68
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	1	0.68
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	10	0.68
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	11	0.68
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD13	18	0.68
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	15	0.68
(1,2284)	2:42:B:ILE:HD13	2:42:B:ILE:H	17	0.68
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	15	0.68
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	16	0.68
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	7	0.68
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	16	0.68
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	4	0.68
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	13	0.68
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	2	0.68
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	12	0.68
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	11	0.68
(1,1873)	1:1626:A:LEU:HD13	1:1628:A:SER:H	18	0.68
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	5	0.68
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	16	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	6	0.68
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	17	0.68
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD11	15	0.68
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	17	0.68
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	20	0.68
(1,1585)	1:1550:A:MET:H	1:1539:A:THR:HG21	8	0.68
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG12	10	0.68
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	14	0.68
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	19	0.68
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG13	18	0.68
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	10	0.68
(1,1201)	1:1587:A:VAL:HG21	1:1584:A:VAL:H	11	0.68
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD21	3	0.68
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	2	0.68
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	3	0.68
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	2	0.68
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	3	0.68
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	8	0.68
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	20	0.68
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	19	0.68
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	5	0.68
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	7	0.68
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD12	3	0.68
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD11	11	0.68
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD21	17	0.68
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD23	19	0.68
(1,636)	1:1588:A:LEU:HD21	1:1529:A:LEU:HD12	3	0.68
(1,622)	1:1644:A:LEU:HD13	1:1532:A:LEU:HD22	5	0.68
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	9	0.68
(1,569)	1:1547:A:VAL:HG12	1:1539:A:THR:HG22	13	0.68
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	18	0.68
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD1	6	0.68
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	9	0.68
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	7	0.68
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD21	1	0.68
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG22	4	0.68
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG13	6	0.68
(1,325)	2:17:B:LEU:HD11	2:28:B:PHE:HB2	19	0.68
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG21	18	0.68
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	19	0.68
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	7	0.68
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	11	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	1	0.68
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	8	0.68
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	17	0.68
(1,267)	2:35:B:VAL:HG23	2:37:B:ARG:HD3	3	0.68
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	1	0.68
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	16	0.68
(1,204)	1:1626:A:LEU:HD11	1:1639:A:SER:H	14	0.68
(1,173)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	20	0.68
(1,125)	1:1591:A:VAL:HG21	1:1592:A:TYR:HB3	19	0.68
(1,124)	1:1613:A:VAL:HG21	1:1611:A:SER:HB2	16	0.68
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	7	0.68
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	12	0.68
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	1	0.68
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	12	0.68
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	20	0.68
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB3	13	0.68
(1,40)	1:1587:A:VAL:HG23	1:1586:A:GLN:HE21	17	0.68
(1,5)	1:1552:A:ILE:HD11	1:1529:A:LEU:HD13	6	0.68
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	14	0.67
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	2	0.67
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG21	3	0.67
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG21	5	0.67
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG21	19	0.67
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	20	0.67
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	13	0.67
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD2	16	0.67
(1,2861)	2:20:B:VAL:HG23	2:19:B:PHE:HD2	4	0.67
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD2	8	0.67
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	3	0.67
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	4	0.67
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	6	0.67
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	17	0.67
(1,2529)	2:43:B:VAL:HG22	2:44:B:GLU:HG3	1	0.67
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	6	0.67
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	17	0.67
(1,2459)	2:56:B:LEU:HD22	2:53:B:LEU:HB2	9	0.67
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG13	4	0.67
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	19	0.67
(1,2445)	2:7:B:THR:HG22	2:50:B:SER:HB3	1	0.67
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	12	0.67
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG21	16	0.67
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD11	15	0.67
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	4	0.67
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	16	0.67
(1,2149)	1:1584:A:VAL:HG12	1:1585:A:ASP:H	15	0.67
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	16	0.67
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG11	1	0.67
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	6	0.67
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	6	0.67
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG13	15	0.67
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	7	0.67
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	9	0.67
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	20	0.67
(1,1753)	1:1605:A:SER:H	1:1604:A:LEU:HD11	9	0.67
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	4	0.67
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	6	0.67
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD23	12	0.67
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	1	0.67
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	10	0.67
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	9	0.67
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD11	1	0.67
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD11	15	0.67
(1,1042)	1:1609:A:VAL:HG12	1:1637:A:PHE:HB3	12	0.67
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	18	0.67
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	17	0.67
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	18	0.67
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	20	0.67
(1,708)	1:1590:A:LEU:HD13	1:1592:A:TYR:HD1	2	0.67
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD12	10	0.67
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD13	16	0.67
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	1	0.67
(1,523)	1:1613:A:VAL:HG21	1:1641:A:HIS:HD2	12	0.67
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD23	17	0.67
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	11	0.67
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	20	0.67
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	2	0.67
(1,290)	2:26:B:PHE:H	2:18:B:GLN:H	7	0.67
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	2	0.67
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	13	0.67
(1,236)	2:20:B:VAL:HG11	2:19:B:PHE:HA	1	0.67
(1,227)	2:17:B:LEU:HD21	2:26:B:PHE:HB2	4	0.67
(1,173)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	7	0.67
(1,125)	1:1591:A:VAL:HG23	1:1582:A:ARG:HD3	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	14	0.67
(1,62)	1:1588:A:LEU:HD12	1:1645:A:ALA:HA	12	0.67
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	1	0.67
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	7	0.67
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	18	0.67
(1,25)	1:1584:A:VAL:HG13	1:1582:A:ARG:HD3	18	0.67
(1,3019)	2:18:B:GLN:HG3	1:1545:A:SER:HB3	7	0.66
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	15	0.66
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG22	15	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG21	2	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	6	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	7	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	8	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	14	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	15	0.66
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	7	0.66
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	11	0.66
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	10	0.66
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	14	0.66
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD22	6	0.66
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	4	0.66
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	3	0.66
(1,2451)	2:62:B:THR:HG21	2:63:B:PRO:HB3	4	0.66
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	6	0.66
(1,2310)	2:20:B:VAL:HG13	2:21:B:CYS:HB3	1	0.66
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD13	9	0.66
(1,2289)	2:42:B:ILE:HD12	2:55:B:LEU:HD13	20	0.66
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA3	11	0.66
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	12	0.66
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	2	0.66
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	4	0.66
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	4	0.66
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	6	0.66
(1,2184)	1:1558:A:ASN:HD21	1:1558:A:ASN:HB2	11	0.66
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	10	0.66
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	17	0.66
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	15	0.66
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG11	18	0.66
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	19	0.66
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	5	0.66
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	4	0.66
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD11	4	0.66
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	2	0.66
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	12	0.66
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	3	0.66
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	19	0.66
(1,1033)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	15	0.66
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	15	0.66
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD22	13	0.66
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD22	17	0.66
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD22	20	0.66
(1,1017)	1:1527:A:PHE:HD2	1:1518:A:VAL:HG21	12	0.66
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	9	0.66
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	18	0.66
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	19	0.66
(1,924)	1:1520:A:ASN:HB3	1:1527:A:PHE:HE1	16	0.66
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	5	0.66
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	15	0.66
(1,693)	1:1590:A:LEU:HD21	1:1592:A:TYR:HA	15	0.66
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	18	0.66
(1,691)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	19	0.66
(1,663)	1:1563:A:VAL:HG22	1:1559:A:CYS:HB2	10	0.66
(1,663)	1:1563:A:VAL:HG23	1:1559:A:CYS:HB2	18	0.66
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	17	0.66
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD23	8	0.66
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	4	0.66
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	12	0.66
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	3	0.66
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD2	6	0.66
(1,561)	1:1587:A:VAL:HG11	1:1589:A:GLN:HE22	18	0.66
(1,480)	1:1627:A:ILE:HG23	1:1626:A:LEU:HD12	4	0.66
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	16	0.66
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	19	0.66
(1,370)	2:18:B:GLN:HG2	1:1542:A:TYR:HD1	17	0.66
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	6	0.66
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	15	0.66
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD23	2	0.66
(1,236)	2:20:B:VAL:HG11	2:19:B:PHE:HA	18	0.66
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	12	0.66
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	8	0.66
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	9	0.66
(1,129)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	1	0.66
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD2	14	0.66
(1,102)	1:1610:A:ILE:HD13	1:1609:A:VAL:H	11	0.66
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	8	0.66
(1,56)	1:1563:A:VAL:HG21	1:1572:A:ILE:H	12	0.66
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	10	0.66
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	12	0.66
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	10	0.65
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	11	0.65
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	16	0.65
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	12	0.65
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE2	13	0.65
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	5	0.65
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB1	11	0.65
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG3	6	0.65
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG21	13	0.65
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	8	0.65
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	2	0.65
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	14	0.65
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	5	0.65
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	10	0.65
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD1	12	0.65
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	13	0.65
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	11	0.65
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	3	0.65
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	11	0.65
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	17	0.65
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	6	0.65
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG12	11	0.65
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	5	0.65
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	13	0.65
(1,1054)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	20	0.65
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	7	0.65
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	15	0.65
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	1	0.65
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	3	0.65
(1,726)	1:1604:A:LEU:HD13	1:1602:A:SER:HA	19	0.65
(1,725)	1:1581:A:LEU:HD22	1:1517:A:GLN:HA	10	0.65
(1,718)	1:1581:A:LEU:HD22	1:1518:A:VAL:HG23	14	0.65
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	4	0.65
(1,693)	1:1590:A:LEU:HD23	1:1592:A:TYR:HA	14	0.65
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD12	1	0.65
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD22	6	0.65
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	15	0.65
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	7	0.65
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG22	3	0.65
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	3	0.65
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD2	18	0.65
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	20	0.65
(1,388)	2:16:B:THR:H	2:12:B:GLU:HG3	15	0.65
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG22	17	0.65
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	8	0.65
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG3	10	0.65
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	5	0.65
(1,287)	2:64:B:ALA:HA	2:63:B:PRO:HB3	16	0.65
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD21	9	0.65
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	10	0.65
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	17	0.65
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	13	0.65
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	11	0.65
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	10	0.65
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	12	0.65
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	15	0.65
(1,173)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	9	0.65
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	15	0.65
(1,129)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	7	0.65
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	17	0.65
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	3	0.65
(1,98)	1:1636:A:LEU:HD21	1:1606:A:TYR:HB2	13	0.65
(1,62)	1:1588:A:LEU:HD12	1:1645:A:ALA:HA	4	0.65
(1,40)	1:1587:A:VAL:HG22	1:1586:A:GLN:HE21	20	0.65
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE1	7	0.65
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	13	0.65
(1,27)	1:1609:A:VAL:HG23	1:1637:A:PHE:HB3	4	0.65
(1,15)	1:1577:A:ALA:HB3	1:1555:A:GLU:HG2	6	0.65
(1,15)	1:1577:A:ALA:HB1	1:1555:A:GLU:HG2	19	0.65
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG23	18	0.64
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD1	15	0.64
(1,2841)	2:13:B:LEU:HD22	2:47:B:CYS:H	10	0.64
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	1	0.64
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	5	0.64
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	12	0.64
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	16	0.64
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	14	0.64
(1,2439)	2:13:B:LEU:HD22	2:47:B:CYS:H	10	0.64
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	14	0.64
(1,2322)	2:32:B:ALA:HB1	2:33:B:SER:HB3	16	0.64
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	8	0.64
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	15	0.64
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD22	6	0.64
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	15	0.64
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD1	3	0.64
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	14	0.64
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE1	15	0.64
(1,2149)	1:1584:A:VAL:HG13	1:1585:A:ASP:H	8	0.64
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG11	8	0.64
(1,2027)	1:1562:A:GLY:H	1:1563:A:VAL:HG12	9	0.64
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	19	0.64
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	12	0.64
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	3	0.64
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	16	0.64
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	17	0.64
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	14	0.64
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	9	0.64
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	15	0.64
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD22	1	0.64
(1,1200)	1:1584:A:VAL:H	1:1518:A:VAL:HG22	12	0.64
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD12	13	0.64
(1,1067)	1:1588:A:LEU:HD11	1:1583:A:TYR:HB3	15	0.64
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	1	0.64
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	10	0.64
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	13	0.64
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	10	0.64
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	1	0.64
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	11	0.64
(1,677)	1:1529:A:LEU:HD12	1:1590:A:LEU:HD11	16	0.64
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	9	0.64
(1,660)	1:1636:A:LEU:HD13	1:1636:A:LEU:HA	4	0.64
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	7	0.64
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	16	0.64
(1,563)	1:1591:A:VAL:HG12	1:1589:A:GLN:HE21	16	0.64
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	16	0.64
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	19	0.64
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	3	0.64
(1,440)	1:1550:A:MET:HE2	1:1638:A:PHE:HD1	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	14	0.64
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	13	0.64
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	14	0.64
(1,236)	2:20:B:VAL:HG11	2:19:B:PHE:HA	7	0.64
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	9	0.64
(1,228)	2:55:B:LEU:HD21	2:46:B:CYS:HA	8	0.64
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	4	0.64
(1,139)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	2	0.64
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	8	0.64
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	10	0.64
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG23	11	0.64
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG22	18	0.64
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	9	0.64
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	13	0.64
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	7	0.64
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	6	0.64
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	5	0.64
(1,3002)	2:42:B:ILE:HD11	2:28:B:PHE:HE2	10	0.63
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	17	0.63
(1,2848)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	19	0.63
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	13	0.63
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD22	1	0.63
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD23	19	0.63
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	4	0.63
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB1	16	0.63
(1,2619)	2:37:B:ARG:H	2:37:B:ARG:HG3	10	0.63
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE1	17	0.63
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	20	0.63
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	18	0.63
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	2	0.63
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	18	0.63
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	7	0.63
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	7	0.63
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	8	0.63
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	12	0.63
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	15	0.63
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	2	0.63
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	2	0.63
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	7	0.63
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	1	0.63
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	7	0.63
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	14	0.63
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	15	0.63
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	15	0.63
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	5	0.63
(1,1324)	1:1577:A:ALA:H	1:1563:A:VAL:HG11	10	0.63
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	7	0.63
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	8	0.63
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	13	0.63
(1,1136)	1:1590:A:LEU:HD23	1:1554:A:GLY:H	9	0.63
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	7	0.63
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD21	8	0.63
(1,1004)	1:1644:A:LEU:HD23	1:1645:A:ALA:H	5	0.63
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	7	0.63
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	8	0.63
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	12	0.63
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	15	0.63
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	12	0.63
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG12	12	0.63
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	14	0.63
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE1	6	0.63
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	9	0.63
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	4	0.63
(1,693)	1:1590:A:LEU:HD21	1:1592:A:TYR:HA	7	0.63
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD11	6	0.63
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD11	9	0.63
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	3	0.63
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	5	0.63
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	20	0.63
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	5	0.63
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	19	0.63
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	5	0.63
(1,523)	1:1613:A:VAL:HG22	1:1641:A:HIS:HD2	18	0.63
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	12	0.63
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	15	0.63
(1,434)	1:1610:A:ILE:HD11	1:1590:A:LEU:HB3	1	0.63
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG22	8	0.63
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	5	0.63
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	10	0.63
(1,317)	2:53:B:LEU:H	2:55:B:LEU:HB3	20	0.63
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	10	0.63
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	13	0.63
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HB3	18	0.63
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	14	0.63
(1,236)	2:20:B:VAL:HG12	2:19:B:PHE:HA	19	0.63
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	10	0.63
(1,226)	2:17:B:LEU:HD11	2:18:B:GLN:HA	14	0.63
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	13	0.63
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	19	0.63
(1,129)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	6	0.63
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	3	0.63
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	1	0.63
(1,98)	1:1636:A:LEU:HD23	1:1606:A:TYR:HB2	3	0.63
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	19	0.63
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	15	0.63
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	3	0.63
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	8	0.63
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	16	0.63
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	1	0.63
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG22	4	0.62
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	1	0.62
(1,2937)	2:20:B:VAL:H	2:20:B:VAL:HG22	12	0.62
(1,2848)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	5	0.62
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	16	0.62
(1,2845)	2:17:B:LEU:HD23	2:26:B:PHE:HD1	6	0.62
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	6	0.62
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	16	0.62
(1,2737)	2:56:B:LEU:H	2:56:B:LEU:HD23	7	0.62
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB1	14	0.62
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	12	0.62
(1,2703)	2:5:B:SER:H	2:4:B:PRO:HB2	12	0.62
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE2	11	0.62
(1,2521)	2:35:B:VAL:HG22	2:33:B:SER:HB3	12	0.62
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD22	2	0.62
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD21	8	0.62
(1,2451)	2:62:B:THR:HG22	2:63:B:PRO:HB3	16	0.62
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	6	0.62
(1,2310)	2:20:B:VAL:HG13	2:21:B:CYS:HB3	18	0.62
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	3	0.62
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	8	0.62
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA2	17	0.62
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	19	0.62
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	18	0.62
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	18	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	6	0.62
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	10	0.62
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	18	0.62
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	19	0.62
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	1	0.62
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	18	0.62
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	5	0.62
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	20	0.62
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	7	0.62
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	15	0.62
(1,1712)	1:1572:A:ILE:HG23	1:1596:A:SER:H	5	0.62
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	3	0.62
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	10	0.62
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	14	0.62
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	18	0.62
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	5	0.62
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	13	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	1	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	4	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	6	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	12	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	14	0.62
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	18	0.62
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	19	0.62
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	10	0.62
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	19	0.62
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	14	0.62
(1,993)	1:1610:A:ILE:HD13	1:1609:A:VAL:HA	16	0.62
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	6	0.62
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	8	0.62
(1,752)	1:1550:A:MET:HG2	1:1548:A:VAL:HG12	4	0.62
(1,708)	1:1590:A:LEU:HD11	1:1592:A:TYR:HD1	17	0.62
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD12	2	0.62
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD22	6	0.62
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	10	0.62
(1,528)	1:1570:A:THR:HG21	1:1571:A:ARG:H	9	0.62
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	11	0.62
(1,520)	1:1541:A:ALA:HB1	1:1542:A:TYR:HD1	7	0.62
(1,406)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	13	0.62
(1,395)	1:1629:A:LEU:HD11	2:19:B:PHE:HD2	13	0.62
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG3	15	0.62
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	17	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	2:54:B:ALA:H	2:55:B:LEU:HD12	15	0.62
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD12	11	0.62
(1,310)	2:43:B:VAL:H	2:45:B:GLU:HB2	10	0.62
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	7	0.62
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	9	0.62
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	16	0.62
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	18	0.62
(1,267)	2:35:B:VAL:HG21	2:34:B:ARG:HD2	11	0.62
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	13	0.62
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	11	0.62
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	17	0.62
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	4	0.62
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	15	0.62
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	19	0.62
(1,49)	1:1540:A:ALA:HB1	1:1625:A:MET:HG2	5	0.62
(1,39)	1:1548:A:VAL:HG23	1:1542:A:TYR:HE2	11	0.62
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	9	0.62
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	19	0.62
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE2	9	0.61
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	20	0.61
(1,2848)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	4	0.61
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD23	14	0.61
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	4	0.61
(1,2817)	2:20:B:VAL:H	2:19:B:PHE:HE2	4	0.61
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	20	0.61
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	1	0.61
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	18	0.61
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	12	0.61
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	5	0.61
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD23	20	0.61
(1,2494)	2:37:B:ARG:HG2	2:37:B:ARG:HA	14	0.61
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	17	0.61
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG11	14	0.61
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	15	0.61
(1,2324)	2:64:B:ALA:HB1	2:63:B:PRO:HA	13	0.61
(1,2292)	2:17:B:LEU:HD13	2:42:B:ILE:HG13	17	0.61
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	7	0.61
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	16	0.61
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	11	0.61
(1,2162)	1:1539:A:THR:HG22	1:1547:A:VAL:H	20	0.61
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	2	0.61
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD22	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	19	0.61
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	12	0.61
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD11	19	0.61
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	14	0.61
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	19	0.61
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG12	18	0.61
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	6	0.61
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	10	0.61
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	11	0.61
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	20	0.61
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	6	0.61
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	15	0.61
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	1	0.61
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	4	0.61
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	11	0.61
(1,1397)	1:1591:A:VAL:HG23	1:1591:A:VAL:H	19	0.61
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	5	0.61
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	11	0.61
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	16	0.61
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	19	0.61
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	6	0.61
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	18	0.61
(1,1117)	1:1574:A:VAL:HG23	1:1608:A:SER:HA	7	0.61
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	1	0.61
(1,1017)	1:1527:A:PHE:HD2	1:1518:A:VAL:HG21	5	0.61
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	17	0.61
(1,806)	1:1584:A:VAL:HG23	1:1585:A:ASP:HB2	16	0.61
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	13	0.61
(1,693)	1:1590:A:LEU:HD21	1:1592:A:TYR:HA	3	0.61
(1,677)	1:1529:A:LEU:HD12	1:1590:A:LEU:HD11	20	0.61
(1,609)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	20	0.61
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	16	0.61
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	12	0.61
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	8	0.61
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	15	0.61
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	18	0.61
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD1	2	0.61
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD1	16	0.61
(1,454)	1:1550:A:MET:HE2	1:1610:A:ILE:HG12	1	0.61
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	19	0.61
(1,380)	2:12:B:GLU:HG2	1:1570:A:THR:HG23	9	0.61
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	12	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	18	0.61
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	15	0.61
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	10	0.61
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	15	0.61
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	3	0.61
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	10	0.61
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	10	0.61
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	14	0.61
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	1	0.61
(1,129)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	14	0.61
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	17	0.61
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	10	0.61
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	13	0.61
(1,66)	1:1636:A:LEU:HD12	1:1638:A:PHE:HZ	11	0.61
(1,47)	1:1518:A:VAL:HG13	1:1513:A:HIS:HB3	20	0.61
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	18	0.61
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	10	0.61
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	13	0.61
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	12	0.6
(1,3016)	2:18:B:GLN:HE22	1:1545:A:SER:HB2	14	0.6
(1,3013)	1:1629:A:LEU:HD12	2:19:B:PHE:HZ	17	0.6
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	15	0.6
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	13	0.6
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	13	0.6
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	1	0.6
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	1	0.6
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	16	0.6
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG2	20	0.6
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	1	0.6
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	3	0.6
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	3	0.6
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD22	12	0.6
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	20	0.6
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	1	0.6
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	16	0.6
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	8	0.6
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	18	0.6
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	10	0.6
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	16	0.6
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG23	17	0.6
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	7	0.6
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	14	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	7	0.6
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	13	0.6
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	17	0.6
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	1	0.6
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	6	0.6
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	11	0.6
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	15	0.6
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	9	0.6
(1,1770)	1:1547:A:VAL:H	1:1549:A:TYR:HE2	1	0.6
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	18	0.6
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	9	0.6
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	9	0.6
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	20	0.6
(1,1627)	1:1558:A:ASN:H	1:1558:A:ASN:HD21	12	0.6
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	15	0.6
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	16	0.6
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	12	0.6
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	20	0.6
(1,1299)	1:1563:A:VAL:HG21	1:1563:A:VAL:H	13	0.6
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	3	0.6
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	9	0.6
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	10	0.6
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG13	17	0.6
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	14	0.6
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	8	0.6
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	13	0.6
(1,1067)	1:1588:A:LEU:HD12	1:1583:A:TYR:HB3	6	0.6
(1,1063)	1:1644:A:LEU:HD11	1:1644:A:LEU:HB3	19	0.6
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	16	0.6
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	8	0.6
(1,1000)	1:1566:A:CYS:HA	1:1563:A:VAL:HG23	4	0.6
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	6	0.6
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	9	0.6
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD11	11	0.6
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	12	0.6
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	6	0.6
(1,745)	1:1601:A:LYS:HD2	1:1601:A:LYS:HA	8	0.6
(1,725)	1:1581:A:LEU:HD21	1:1517:A:GLN:HA	3	0.6
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	16	0.6
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	2	0.6
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	3	0.6
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:1547:A:VAL:HG12	1:1539:A:THR:HG22	16	0.6
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	11	0.6
(1,523)	1:1613:A:VAL:HG21	1:1641:A:HIS:HD2	4	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	2	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	6	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	9	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	14	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	17	0.6
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	19	0.6
(1,494)	1:1610:A:ILE:HG22	1:1638:A:PHE:HD2	1	0.6
(1,433)	1:1610:A:ILE:HD12	1:1610:A:ILE:HB	1	0.6
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	1	0.6
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	18	0.6
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG22	2	0.6
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	9	0.6
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD11	19	0.6
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	6	0.6
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	20	0.6
(1,270)	2:56:B:LEU:HD23	1:1600:A:SER:H	3	0.6
(1,204)	1:1610:A:ILE:HG22	1:1639:A:SER:H	20	0.6
(1,185)	1:1632:A:GLN:H	1:1629:A:LEU:HD13	3	0.6
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	15	0.6
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD3	13	0.6
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	14	0.6
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	20	0.6
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG23	4	0.6
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	9	0.6
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	2	0.6
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	16	0.6
(1,10)	1:1550:A:MET:HE3	1:1549:A:TYR:HA	15	0.6
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG12	13	0.59
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG11	20	0.59
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD22	6	0.59
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	1	0.59
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG13	2	0.59
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	2	0.59
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	12	0.59
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD23	14	0.59
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB1	12	0.59
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG2	5	0.59
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	12	0.59
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	17	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD22	13	0.59
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	16	0.59
(1,2418)	2:63:B:PRO:HD3	2:63:B:PRO:HB3	13	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	5	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	6	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	11	0.59
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	18	0.59
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD11	13	0.59
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	10	0.59
(1,2281)	2:42:B:ILE:HD12	2:59:B:TYR:HB3	6	0.59
(1,2232)	1:1567:A:PHE:HD2	1:1542:A:TYR:HE2	7	0.59
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	12	0.59
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	9	0.59
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	13	0.59
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	8	0.59
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	13	0.59
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	19	0.59
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	2	0.59
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	12	0.59
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	3	0.59
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	19	0.59
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG21	1	0.59
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	20	0.59
(1,1397)	1:1591:A:VAL:HG21	1:1591:A:VAL:H	6	0.59
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	1	0.59
(1,1299)	1:1563:A:VAL:HG22	1:1563:A:VAL:H	7	0.59
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	15	0.59
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG12	20	0.59
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	16	0.59
(1,1108)	1:1583:A:TYR:HD1	1:1585:A:ASP:HA	6	0.59
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	12	0.59
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HD1	15	0.59
(1,1003)	1:1644:A:LEU:HD22	1:1532:A:LEU:H	7	0.59
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	5	0.59
(1,993)	1:1610:A:ILE:HD12	1:1609:A:VAL:HA	11	0.59
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	12	0.59
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	18	0.59
(1,745)	1:1601:A:LYS:HD2	1:1601:A:LYS:HA	14	0.59
(1,725)	1:1581:A:LEU:HD21	1:1517:A:GLN:HA	17	0.59
(1,715)	1:1604:A:LEU:HD21	1:1603:A:GLY:HA2	3	0.59
(1,711)	1:1604:A:LEU:HD22	1:1605:A:SER:H	13	0.59
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD11	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:1635:A:THR:HG22	1:1607:A:LYS:HG3	2	0.59
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	13	0.59
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	4	0.59
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	8	0.59
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	20	0.59
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD2	14	0.59
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	4	0.59
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	7	0.59
(1,524)	1:1577:A:ALA:HB1	1:1592:A:TYR:HE1	9	0.59
(1,523)	1:1613:A:VAL:HG22	1:1641:A:HIS:HD2	5	0.59
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	5	0.59
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	7	0.59
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	8	0.59
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	11	0.59
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD12	10	0.59
(1,396)	1:1542:A:TYR:HD2	2:19:B:PHE:HD1	2	0.59
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	3	0.59
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	9	0.59
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	16	0.59
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG23	9	0.59
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	2	0.59
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	20	0.59
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	9	0.59
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	18	0.59
(1,234)	2:55:B:LEU:HD13	2:58:B:THR:HG21	2	0.59
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	8	0.59
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	12	0.59
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	11	0.59
(1,226)	2:17:B:LEU:HD12	2:18:B:GLN:HA	7	0.59
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	2	0.59
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	2	0.59
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	3	0.59
(1,129)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	17	0.59
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	11	0.59
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	18	0.59
(1,59)	1:1590:A:LEU:HD21	1:1578:A:ASN:HB2	3	0.59
(1,30)	1:1587:A:VAL:HG21	1:1585:A:ASP:H	11	0.59
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	19	0.59
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	14	0.59
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	17	0.59
(1,27)	1:1609:A:VAL:HG21	1:1637:A:PHE:HB3	8	0.59
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	17	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD22	1	0.58
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	5	0.58
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG22	1	0.58
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	7	0.58
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	11	0.58
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB1	10	0.58
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD22	6	0.58
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD23	19	0.58
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	17	0.58
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	11	0.58
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	6	0.58
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD22	1	0.58
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD23	10	0.58
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	11	0.58
(1,2443)	2:63:B:PRO:HD3	2:62:B:THR:HG22	20	0.58
(1,2382)	2:55:B:LEU:HD23	2:51:B:CYS:HA	6	0.58
(1,2364)	2:44:B:GLU:HG3	2:48:B:PHE:HB2	7	0.58
(1,2339)	2:18:B:GLN:HG3	2:26:B:PHE:HD1	19	0.58
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	17	0.58
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	17	0.58
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	13	0.58
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	16	0.58
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	17	0.58
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	20	0.58
(1,2274)	2:14:B:VAL:HG23	2:18:B:GLN:HG3	5	0.58
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	8	0.58
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	11	0.58
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	20	0.58
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	4	0.58
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	11	0.58
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	16	0.58
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	6	0.58
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG13	12	0.58
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	7	0.58
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	11	0.58
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	16	0.58
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	20	0.58
(1,1712)	1:1572:A:ILE:HG22	1:1596:A:SER:H	4	0.58
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	2	0.58
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	8	0.58
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	16	0.58
(1,1589)	1:1604:A:LEU:H	1:1604:A:LEU:HD11	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	2	0.58
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	11	0.58
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	9	0.58
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	5	0.58
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	9	0.58
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	13	0.58
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	4	0.58
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	14	0.58
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	3	0.58
(1,1201)	1:1587:A:VAL:HG21	1:1584:A:VAL:H	7	0.58
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	15	0.58
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	5	0.58
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	3	0.58
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	13	0.58
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	13	0.58
(1,1114)	1:1583:A:TYR:HE1	1:1585:A:ASP:HA	6	0.58
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	2	0.58
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	2	0.58
(1,1003)	1:1644:A:LEU:HD22	1:1532:A:LEU:H	16	0.58
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD11	2	0.58
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	12	0.58
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	2	0.58
(1,795)	1:1617:A:GLU:HG3	1:1617:A:GLU:H	16	0.58
(1,745)	1:1601:A:LYS:HD2	1:1601:A:LYS:HA	18	0.58
(1,725)	1:1581:A:LEU:HD21	1:1517:A:GLN:HA	4	0.58
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	19	0.58
(1,725)	1:1581:A:LEU:HD21	1:1517:A:GLN:HA	20	0.58
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	17	0.58
(1,652)	1:1581:A:LEU:HD12	1:1527:A:PHE:HD2	10	0.58
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD22	18	0.58
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD2	6	0.58
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	3	0.58
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	5	0.58
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	7	0.58
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	14	0.58
(1,584)	1:1540:A:ALA:HB2	1:1638:A:PHE:HD1	9	0.58
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	5	0.58
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	17	0.58
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	1	0.58
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD2	11	0.58
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	6	0.58
(1,451)	1:1550:A:MET:HE1	1:1610:A:ILE:HG13	16	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:1610:A:ILE:HD12	1:1610:A:ILE:HB	6	0.58
(1,424)	1:1552:A:ILE:HD12	1:1592:A:TYR:HH	15	0.58
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	6	0.58
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	19	0.58
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	13	0.58
(1,317)	2:53:B:LEU:H	1:1601:A:LYS:HB2	17	0.58
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	18	0.58
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA2	1	0.58
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	6	0.58
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD1	15	0.58
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	5	0.58
(1,270)	2:56:B:LEU:HD21	1:1600:A:SER:H	19	0.58
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	5	0.58
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	2	0.58
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	11	0.58
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	15	0.58
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	8	0.58
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG21	8	0.58
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	18	0.58
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	20	0.58
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	4	0.58
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	1	0.58
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	5	0.58
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	2	0.58
(1,91)	1:1619:A:GLY:HA2	1:1620:A:PRO:HB3	12	0.58
(1,89)	1:1511:A:ASN:HB3	1:1521:A:PRO:HG3	4	0.58
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	5	0.58
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	20	0.58
(1,34)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	2	0.58
(1,27)	1:1609:A:VAL:HG23	1:1637:A:PHE:HB3	20	0.58
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	12	0.57
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD1	3	0.57
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG21	2	0.57
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	8	0.57
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB1	3	0.57
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	7	0.57
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	12	0.57
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG23	14	0.57
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	4	0.57
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG3	3	0.57
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG3	18	0.57
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD21	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD23	9	0.57
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	15	0.57
(1,2440)	2:17:B:LEU:HD22	2:17:B:LEU:HA	17	0.57
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	13	0.57
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA3	13	0.57
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	19	0.57
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	19	0.57
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	17	0.57
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	7	0.57
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	20	0.57
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG13	18	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	1	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	4	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	5	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	6	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	10	0.57
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	12	0.57
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	15	0.57
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	18	0.57
(1,1578)	1:1644:A:LEU:H	1:1644:A:LEU:HB2	20	0.57
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	20	0.57
(1,1110)	1:1583:A:TYR:HD2	1:1584:A:VAL:HG22	11	0.57
(1,1089)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	15	0.57
(1,1021)	1:1610:A:ILE:HD11	1:1590:A:LEU:HD23	9	0.57
(1,996)	1:1610:A:ILE:HD11	1:1550:A:MET:HG2	18	0.57
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	5	0.57
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG12	10	0.57
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	8	0.57
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	8	0.57
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD22	7	0.57
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	3	0.57
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	11	0.57
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	10	0.57
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD2	12	0.57
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	8	0.57
(1,523)	1:1613:A:VAL:HG21	1:1641:A:HIS:HD2	19	0.57
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	10	0.57
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG12	16	0.57
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	14	0.57
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB1	16	0.57
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	20	0.57
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	16	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	16	0.57
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD2	18	0.57
(1,268)	2:56:B:LEU:HD23	2:55:B:LEU:HG	2	0.57
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	3	0.57
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	6	0.57
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	4	0.57
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	16	0.57
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	10	0.57
(1,129)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	16	0.57
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	2	0.57
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	19	0.57
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	18	0.57
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	9	0.57
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	14	0.57
(1,71)	1:1550:A:MET:HG2	1:1548:A:VAL:HG12	4	0.57
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	10	0.57
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	6	0.57
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	2	0.57
(1,18)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	16	0.57
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	12	0.56
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	10	0.56
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	17	0.56
(1,2984)	2:20:B:VAL:HA	2:20:B:VAL:HG22	4	0.56
(1,2984)	2:20:B:VAL:HA	2:20:B:VAL:HG23	9	0.56
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD2	9	0.56
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD2	20	0.56
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	4	0.56
(1,2861)	2:20:B:VAL:HG23	2:19:B:PHE:HD2	2	0.56
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	7	0.56
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	9	0.56
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	15	0.56
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	18	0.56
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	20	0.56
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB1	10	0.56
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG3	4	0.56
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG2	7	0.56
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG3	2	0.56
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD21	16	0.56
(1,2481)	2:13:B:LEU:HD11	2:14:B:VAL:HB	11	0.56
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG13	12	0.56
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	10	0.56
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	2	0.56
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	9	0.56
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG21	15	0.56
(1,2278)	2:42:B:ILE:HD13	2:55:B:LEU:HB3	5	0.56
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	8	0.56
(1,2273)	2:14:B:VAL:HG23	2:26:B:PHE:HB2	3	0.56
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD2	4	0.56
(1,2162)	1:1539:A:THR:HG23	1:1547:A:VAL:H	6	0.56
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD21	16	0.56
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	7	0.56
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	17	0.56
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	14	0.56
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	15	0.56
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	17	0.56
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	17	0.56
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	5	0.56
(1,1397)	1:1591:A:VAL:HG22	1:1591:A:VAL:H	7	0.56
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	6	0.56
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	18	0.56
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	2	0.56
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	6	0.56
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	4	0.56
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	18	0.56
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	8	0.56
(1,1031)	1:1577:A:ALA:HB3	1:1562:A:GLY:HA3	20	0.56
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	2	0.56
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	6	0.56
(1,993)	1:1610:A:ILE:HD11	1:1609:A:VAL:HA	4	0.56
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	15	0.56
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	20	0.56
(1,795)	1:1617:A:GLU:HG2	1:1617:A:GLU:H	5	0.56
(1,725)	1:1581:A:LEU:HD22	1:1517:A:GLN:HA	7	0.56
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	20	0.56
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD11	10	0.56
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	6	0.56
(1,619)	1:1626:A:LEU:HD22	1:1629:A:LEU:HD12	18	0.56
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	2	0.56
(1,585)	1:1519:A:THR:HG22	1:1520:A:ASN:HD21	19	0.56
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	13	0.56
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	2	0.56
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	13	0.56
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	17	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG13	4	0.56
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	20	0.56
(1,504)	1:1618:A:ALA:HB2	1:1619:A:GLY:HA2	10	0.56
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD2	14	0.56
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	1	0.56
(1,325)	2:17:B:LEU:HD13	2:28:B:PHE:HB2	9	0.56
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	14	0.56
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	10	0.56
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	12	0.56
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	20	0.56
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	9	0.56
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD22	19	0.56
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	19	0.56
(1,208)	1:1609:A:VAL:HG12	1:1590:A:LEU:H	12	0.56
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	12	0.56
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	9	0.56
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	17	0.56
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	6	0.56
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	12	0.56
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	16	0.56
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	18	0.56
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	5	0.56
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	3	0.55
(1,2984)	2:20:B:VAL:HA	2:20:B:VAL:HG23	13	0.55
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	11	0.55
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	19	0.55
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG22	11	0.55
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	14	0.55
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	20	0.55
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	1	0.55
(1,2619)	2:37:B:ARG:H	2:37:B:ARG:HG3	20	0.55
(1,2535)	2:61:B:ALA:HB1	2:27:B:TYR:H	14	0.55
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG3	7	0.55
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	11	0.55
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE2	4	0.55
(1,2515)	2:55:B:LEU:HD21	2:46:B:CYS:HA	8	0.55
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	8	0.55
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG12	17	0.55
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG22	11	0.55
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	11	0.55
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	19	0.55
(1,2418)	2:63:B:PRO:HD3	2:63:B:PRO:HB3	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2418)	2:63:B:PRO:HD3	2:63:B:PRO:HB3	20	0.55
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG11	10	0.55
(1,2382)	2:55:B:LEU:HD21	2:51:B:CYS:HA	14	0.55
(1,2376)	2:42:B:ILE:HG23	2:28:B:PHE:HB3	17	0.55
(1,2322)	2:32:B:ALA:HB3	2:33:B:SER:HB3	5	0.55
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	14	0.55
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	6	0.55
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	18	0.55
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	1	0.55
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	11	0.55
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	13	0.55
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	17	0.55
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	16	0.55
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	20	0.55
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	9	0.55
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	13	0.55
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	10	0.55
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	16	0.55
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD21	19	0.55
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	4	0.55
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	7	0.55
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG22	8	0.55
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	6	0.55
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	13	0.55
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	3	0.55
(1,1350)	1:1622:A:ASN:H	1:1623:A:ARG:HB2	19	0.55
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	4	0.55
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	19	0.55
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	3	0.55
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	16	0.55
(1,1285)	1:1609:A:VAL:H	1:1609:A:VAL:HG11	2	0.55
(1,1228)	1:1642:A:THR:HG22	1:1640:A:TRP:HE1	20	0.55
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	18	0.55
(1,1089)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	9	0.55
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE1	14	0.55
(1,1033)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	7	0.55
(1,1033)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	14	0.55
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	8	0.55
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	7	0.55
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	18	0.55
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	18	0.55
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	7	0.55
(1,725)	1:1581:A:LEU:HD22	1:1517:A:GLN:HA	18	0.55
(1,724)	1:1581:A:LEU:HD22	1:1588:A:LEU:HA	11	0.55
(1,664)	1:1607:A:LYS:HG3	1:1607:A:LYS:HE3	11	0.55
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	14	0.55
(1,585)	1:1519:A:THR:HG21	1:1520:A:ASN:HD21	17	0.55
(1,523)	1:1613:A:VAL:HG23	1:1641:A:HIS:HD2	16	0.55
(1,522)	1:1613:A:VAL:H	1:1613:A:VAL:HG11	13	0.55
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD12	19	0.55
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	5	0.55
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	10	0.55
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	15	0.55
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	19	0.55
(1,301)	2:38:B:ARG:H	2:33:B:SER:HB3	20	0.55
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	8	0.55
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	6	0.55
(1,268)	2:56:B:LEU:HD21	2:55:B:LEU:HG	14	0.55
(1,266)	2:62:B:THR:HG23	2:63:B:PRO:HG3	10	0.55
(1,226)	2:17:B:LEU:HD12	2:18:B:GLN:HA	16	0.55
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	11	0.55
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	11	0.55
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	8	0.55
(1,129)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	9	0.55
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	2	0.55
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	8	0.55
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	12	0.55
(1,76)	1:1544:A:LYS:HB2	1:1543:A:SER:HB3	8	0.55
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	2	0.55
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	11	0.55
(1,17)	1:1577:A:ALA:HB1	1:1553:A:CYS:H	2	0.55
(1,11)	1:1625:A:MET:HE3	1:1624:A:PRO:HA	10	0.55
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	8	0.55
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	20	0.54
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	7	0.54
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE1	12	0.54
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	4	0.54
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	2	0.54
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	19	0.54
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD21	3	0.54
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	1	0.54
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	9	0.54
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	4	0.54
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	6	0.54
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	13	0.54
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	19	0.54
(1,2282)	2:42:B:ILE:HD13	2:42:B:ILE:HA	5	0.54
(1,2273)	2:14:B:VAL:HG21	2:26:B:PHE:HB2	1	0.54
(1,2273)	2:14:B:VAL:HG23	2:26:B:PHE:HB2	16	0.54
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG23	8	0.54
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	6	0.54
(1,2149)	1:1584:A:VAL:HG11	1:1585:A:ASP:H	9	0.54
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	17	0.54
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG11	19	0.54
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	8	0.54
(1,1712)	1:1572:A:ILE:HG23	1:1596:A:SER:H	6	0.54
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	6	0.54
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	18	0.54
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	11	0.54
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	12	0.54
(1,1586)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	1	0.54
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	3	0.54
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	5	0.54
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	7	0.54
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	17	0.54
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	2	0.54
(1,1201)	1:1587:A:VAL:HG21	1:1584:A:VAL:H	13	0.54
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	7	0.54
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	10	0.54
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	1	0.54
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	3	0.54
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	17	0.54
(1,1063)	1:1644:A:LEU:HD13	1:1644:A:LEU:HB3	11	0.54
(1,1021)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD23	19	0.54
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	13	0.54
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	10	0.54
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	16	0.54
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	18	0.54
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	17	0.54
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	8	0.54
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	9	0.54
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	8	0.54
(1,725)	1:1581:A:LEU:HD22	1:1517:A:GLN:HA	11	0.54
(1,711)	1:1604:A:LEU:HD23	1:1605:A:SER:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD13	7	0.54
(1,490)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	1	0.54
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	11	0.54
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	12	0.54
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD12	8	0.54
(1,434)	1:1610:A:ILE:HD13	1:1590:A:LEU:HB3	6	0.54
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	18	0.54
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	3	0.54
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD21	20	0.54
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	16	0.54
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	2	0.54
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD21	12	0.54
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	6	0.54
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	16	0.54
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD1	2	0.54
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	6	0.54
(1,270)	2:56:B:LEU:HD22	1:1600:A:SER:H	15	0.54
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD2	13	0.54
(1,248)	2:29:B:SER:HB3	2:30:B:ARG:HG3	1	0.54
(1,234)	2:55:B:LEU:HD11	2:58:B:THR:HG23	6	0.54
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	5	0.54
(1,205)	1:1612:A:PHE:H	1:1587:A:VAL:HB	16	0.54
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	7	0.54
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	19	0.54
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	20	0.54
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	9	0.54
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	13	0.54
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG21	8	0.54
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	9	0.54
(1,50)	1:1635:A:THR:HG21	1:1609:A:VAL:HB	7	0.54
(1,34)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	1	0.54
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	3	0.54
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	6	0.54
(1,30)	1:1587:A:VAL:HG21	1:1585:A:ASP:H	13	0.54
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	4	0.54
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	17	0.53
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	8	0.53
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD2	6	0.53
(1,2884)	2:43:B:VAL:HG22	2:28:B:PHE:HD2	13	0.53
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	8	0.53
(1,2844)	2:59:B:TYR:HE2	2:42:B:ILE:H	7	0.53
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG21	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	20	0.53
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG21	19	0.53
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	17	0.53
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG3	12	0.53
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE1	8	0.53
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	4	0.53
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	13	0.53
(1,2501)	2:56:B:LEU:HD11	2:20:B:VAL:HG13	4	0.53
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	15	0.53
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	6	0.53
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	8	0.53
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG22	8	0.53
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	12	0.53
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	16	0.53
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	14	0.53
(1,2376)	2:42:B:ILE:HG22	2:28:B:PHE:HB3	20	0.53
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG23	12	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	2	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	15	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	18	0.53
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	20	0.53
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	14	0.53
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	1	0.53
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG22	6	0.53
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	18	0.53
(1,2043)	1:1645:A:ALA:H	1:1646:A:CYS:HB3	17	0.53
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	17	0.53
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	13	0.53
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD11	6	0.53
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	10	0.53
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	11	0.53
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	11	0.53
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	10	0.53
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	10	0.53
(1,1697)	1:1644:A:LEU:HD11	1:1645:A:ALA:H	11	0.53
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	4	0.53
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD23	14	0.53
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	19	0.53
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	10	0.53
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	7	0.53
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	18	0.53
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:1644:A:LEU:H	1:1644:A:LEU:HB2	5	0.53
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG21	4	0.53
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	6	0.53
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	16	0.53
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	7	0.53
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	10	0.53
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	16	0.53
(1,1299)	1:1563:A:VAL:HG23	1:1563:A:VAL:H	6	0.53
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	4	0.53
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	16	0.53
(1,1189)	1:1627:A:ILE:HG12	1:1627:A:ILE:H	15	0.53
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	16	0.53
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	20	0.53
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	4	0.53
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	12	0.53
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	11	0.53
(1,1136)	1:1590:A:LEU:HD23	1:1554:A:GLY:H	14	0.53
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD13	3	0.53
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	4	0.53
(1,1003)	1:1644:A:LEU:HD21	1:1532:A:LEU:H	14	0.53
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	11	0.53
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	13	0.53
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	2	0.53
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	19	0.53
(1,697)	1:1644:A:LEU:HD12	1:1529:A:LEU:HD12	11	0.53
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD12	4	0.53
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD11	13	0.53
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	3	0.53
(1,652)	1:1581:A:LEU:HD13	1:1527:A:PHE:HD2	14	0.53
(1,585)	1:1519:A:THR:HG23	1:1520:A:ASN:HD21	18	0.53
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE1	7	0.53
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	18	0.53
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	14	0.53
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	6	0.53
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	8	0.53
(1,505)	1:1618:A:ALA:HB2	1:1616:A:PRO:HD2	17	0.53
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	3	0.53
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	4	0.53
(1,454)	1:1550:A:MET:HE2	1:1610:A:ILE:HG12	6	0.53
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	17	0.53
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE2	16	0.53
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:1569:A:GLN:HE21	1:1570:A:THR:HG21	9	0.53
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	3	0.53
(1,329)	2:59:B:TYR:HD2	2:58:B:THR:H	7	0.53
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	6	0.53
(1,317)	2:53:B:LEU:H	1:1601:A:LYS:HB2	15	0.53
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD11	15	0.53
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD22	19	0.53
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD2	13	0.53
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	6	0.53
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD22	9	0.53
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	9	0.53
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	10	0.53
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG12	3	0.53
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	17	0.53
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	8	0.53
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	7	0.53
(1,120)	1:1637:A:PHE:HB3	1:1609:A:VAL:HG23	20	0.53
(1,102)	1:1610:A:ILE:HD11	1:1609:A:VAL:H	17	0.53
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	16	0.53
(1,48)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	4	0.53
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	14	0.53
(1,34)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	7	0.53
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	15	0.53
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	1	0.53
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	4	0.52
(1,2987)	2:42:B:ILE:HD13	2:56:B:LEU:HG	20	0.52
(1,2975)	2:17:B:LEU:HD12	2:17:B:LEU:HB3	5	0.52
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG13	1	0.52
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG13	7	0.52
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	12	0.52
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG13	18	0.52
(1,2922)	2:61:B:ALA:HA	2:27:B:TYR:HD1	13	0.52
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	14	0.52
(1,2822)	2:59:B:TYR:H	2:59:B:TYR:HE2	20	0.52
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD22	10	0.52
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	14	0.52
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	7	0.52
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	3	0.52
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB2	15	0.52
(1,2537)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	19	0.52
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	16	0.52
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD23	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	3	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	7	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	13	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	14	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	19	0.52
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	20	0.52
(1,2316)	2:43:B:VAL:H	2:43:B:VAL:HG22	4	0.52
(1,2315)	2:43:B:VAL:HG21	2:40:B:ARG:HD2	18	0.52
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	1	0.52
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	3	0.52
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	10	0.52
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG12	16	0.52
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD13	17	0.52
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	12	0.52
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	13	0.52
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA2	4	0.52
(1,2247)	1:1583:A:TYR:HE1	1:1520:A:ASN:H	12	0.52
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	20	0.52
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	5	0.52
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG21	13	0.52
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	20	0.52
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD21	12	0.52
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	19	0.52
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	2	0.52
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	7	0.52
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	6	0.52
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	17	0.52
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	6	0.52
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	16	0.52
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	8	0.52
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	10	0.52
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	12	0.52
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	12	0.52
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	20	0.52
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	10	0.52
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	14	0.52
(1,1299)	1:1563:A:VAL:HG21	1:1563:A:VAL:H	17	0.52
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	1	0.52
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	17	0.52
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	13	0.52
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	7	0.52
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG11	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	10	0.52
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	19	0.52
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	16	0.52
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	20	0.52
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	3	0.52
(1,904)	1:1601:A:LYS:HG2	1:1602:A:SER:HB3	1	0.52
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	6	0.52
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	1	0.52
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	11	0.52
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	12	0.52
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	19	0.52
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	2	0.52
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	17	0.52
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	14	0.52
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	18	0.52
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD13	3	0.52
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	13	0.52
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE2	4	0.52
(1,480)	1:1627:A:ILE:HG21	1:1626:A:LEU:HD12	20	0.52
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	8	0.52
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD12	6	0.52
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	9	0.52
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	4	0.52
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	6	0.52
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	12	0.52
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	4	0.52
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE2	17	0.52
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	11	0.52
(1,201)	1:1568:A:GLY:H	1:1569:A:GLN:HG3	15	0.52
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	10	0.52
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	1	0.52
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	14	0.52
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	15	0.52
(1,97)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	2	0.52
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	18	0.52
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	8	0.52
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	10	0.52
(1,32)	1:1547:A:VAL:HG23	1:1549:A:TYR:HB3	15	0.52
(1,11)	1:1625:A:MET:HE3	1:1626:A:LEU:HA	18	0.52
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD11	3	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	6	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	10	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	15	0.51
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	19	0.51
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG22	19	0.51
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	13	0.51
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	9	0.51
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	17	0.51
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	8	0.51
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	19	0.51
(1,2481)	2:13:B:LEU:HD11	2:14:B:VAL:HB	3	0.51
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	2	0.51
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	18	0.51
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG22	5	0.51
(1,2425)	2:7:B:THR:H	2:6:B:GLU:HG2	19	0.51
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	5	0.51
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	11	0.51
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	12	0.51
(1,2305)	2:20:B:VAL:HG11	2:17:B:LEU:HA	4	0.51
(1,2284)	2:42:B:ILE:HD11	2:42:B:ILE:H	3	0.51
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	4	0.51
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	4	0.51
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	2	0.51
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	9	0.51
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG12	11	0.51
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD23	10	0.51
(1,1789)	1:1577:A:ALA:HB2	1:1578:A:ASN:H	1	0.51
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD21	8	0.51
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	16	0.51
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	16	0.51
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	2	0.51
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	3	0.51
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	7	0.51
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD12	19	0.51
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	12	0.51
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	3	0.51
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	17	0.51
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	6	0.51
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	9	0.51
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	10	0.51
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	5	0.51
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	1	0.51
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	18	0.51
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	20	0.51
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG11	1	0.51
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG11	18	0.51
(1,1299)	1:1563:A:VAL:HG22	1:1563:A:VAL:H	12	0.51
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	10	0.51
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	2	0.51
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	20	0.51
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	2	0.51
(1,1033)	1:1645:A:ALA:HB1	1:1614:A:CYS:HB3	8	0.51
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	3	0.51
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	13	0.51
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	3	0.51
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	5	0.51
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	10	0.51
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	10	0.51
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	18	0.51
(1,795)	1:1617:A:GLU:HG3	1:1617:A:GLU:H	6	0.51
(1,795)	1:1617:A:GLU:HG3	1:1617:A:GLU:H	12	0.51
(1,714)	1:1604:A:LEU:HD12	1:1604:A:LEU:HA	13	0.51
(1,691)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	11	0.51
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	9	0.51
(1,529)	1:1584:A:VAL:HG12	1:1583:A:TYR:HD1	14	0.51
(1,439)	1:1550:A:MET:HE2	1:1638:A:PHE:HE2	18	0.51
(1,431)	1:1552:A:ILE:HD11	1:1610:A:ILE:HG13	9	0.51
(1,406)	1:1629:A:LEU:HD13	2:19:B:PHE:HD1	5	0.51
(1,395)	1:1629:A:LEU:HD13	2:19:B:PHE:HD1	5	0.51
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG3	12	0.51
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG21	16	0.51
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	8	0.51
(1,297)	2:37:B:ARG:H	2:33:B:SER:HB2	13	0.51
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	13	0.51
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	6	0.51
(1,209)	1:1585:A:ASP:H	1:1586:A:GLN:HB3	7	0.51
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	5	0.51
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	7	0.51
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	4	0.51
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	1	0.51
(1,123)	1:1523:A:THR:HG23	1:1522:A:SER:HB3	9	0.51
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	2	0.51
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	12	0.51
(1,34)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	2:17:B:LEU:HD11	2:17:B:LEU:HB3	17	0.5
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	2	0.5
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	3	0.5
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	14	0.5
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	20	0.5
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG22	6	0.5
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	14	0.5
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	3	0.5
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	19	0.5
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	16	0.5
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	11	0.5
(1,2506)	2:56:B:LEU:HD13	2:20:B:VAL:H	7	0.5
(1,2500)	2:56:B:LEU:HD23	2:55:B:LEU:HD21	5	0.5
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG13	3	0.5
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG21	4	0.5
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	17	0.5
(1,2447)	2:58:B:THR:HA	2:58:B:THR:HG23	18	0.5
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG11	9	0.5
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	19	0.5
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	3	0.5
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	14	0.5
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	6	0.5
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	20	0.5
(1,2162)	1:1548:A:VAL:HG23	1:1547:A:VAL:H	4	0.5
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	3	0.5
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG21	14	0.5
(1,1848)	1:1539:A:THR:HG23	1:1539:A:THR:H	6	0.5
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	7	0.5
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	16	0.5
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	8	0.5
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	1	0.5
(1,1760)	1:1532:A:LEU:HD21	1:1533:A:SER:H	1	0.5
(1,1760)	1:1532:A:LEU:HD21	1:1533:A:SER:H	3	0.5
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	2	0.5
(1,1712)	1:1572:A:ILE:HG22	1:1596:A:SER:H	9	0.5
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	12	0.5
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	5	0.5
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	9	0.5
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	19	0.5
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD11	3	0.5
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD23	3	0.5
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	16	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	14	0.5
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	4	0.5
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	3	0.5
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	4	0.5
(1,1355)	1:1621:A:THR:HG22	1:1622:A:ASN:H	9	0.5
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	11	0.5
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	5	0.5
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	14	0.5
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	15	0.5
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	19	0.5
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	4	0.5
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	6	0.5
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	9	0.5
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	11	0.5
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	12	0.5
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	9	0.5
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	10	0.5
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	15	0.5
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	12	0.5
(1,1005)	1:1532:A:LEU:HD22	1:1612:A:PHE:HZ	1	0.5
(1,1005)	1:1532:A:LEU:HD22	1:1612:A:PHE:HZ	6	0.5
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	14	0.5
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	2	0.5
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	13	0.5
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	19	0.5
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG21	10	0.5
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	20	0.5
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD13	4	0.5
(1,660)	1:1636:A:LEU:HD12	1:1636:A:LEU:HA	12	0.5
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	17	0.5
(1,586)	1:1548:A:VAL:HG21	1:1638:A:PHE:HD2	16	0.5
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	15	0.5
(1,528)	1:1570:A:THR:HG21	1:1571:A:ARG:H	10	0.5
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	7	0.5
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	5	0.5
(1,483)	1:1610:A:ILE:HG21	1:1590:A:LEU:HB3	8	0.5
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD22	18	0.5
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	17	0.5
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	20	0.5
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	19	0.5
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	3	0.5
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	13	0.5
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	7	0.5
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	15	0.5
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	17	0.5
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	1	0.5
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB3	12	0.5
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	18	0.5
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD2	12	0.5
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	14	0.5
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	20	0.5
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	16	0.5
(1,129)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	13	0.5
(1,124)	1:1613:A:VAL:HG22	1:1611:A:SER:HB2	19	0.5
(1,105)	1:1548:A:VAL:HG21	1:1550:A:MET:HB3	4	0.5
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	4	0.5
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	3	0.5
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	10	0.5
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	4	0.5
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	5	0.49
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	13	0.49
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	8	0.49
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	5	0.49
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG12	17	0.49
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	8	0.49
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	9	0.49
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD12	9	0.49
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD12	17	0.49
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG21	1	0.49
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	12	0.49
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	14	0.49
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB2	6	0.49
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	8	0.49
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	15	0.49
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG2	20	0.49
(1,2501)	2:56:B:LEU:HD13	2:20:B:VAL:HG13	9	0.49
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	14	0.49
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	19	0.49
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG12	1	0.49
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG13	19	0.49
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	6	0.49
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	19	0.49
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	11	0.49
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	8	0.49
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD11	1	0.49
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	2	0.49
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD11	7	0.49
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	10	0.49
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD22	3	0.49
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	12	0.49
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	5	0.49
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	16	0.49
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG11	8	0.49
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG12	15	0.49
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB2	13	0.49
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	7	0.49
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	18	0.49
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	20	0.49
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	3	0.49
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	11	0.49
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	14	0.49
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD11	13	0.49
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	2	0.49
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	6	0.49
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	14	0.49
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	15	0.49
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	10	0.49
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	5	0.49
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	19	0.49
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	6	0.49
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	8	0.49
(1,1228)	1:1642:A:THR:HG21	1:1640:A:TRP:HE1	1	0.49
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	8	0.49
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	15	0.49
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	19	0.49
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	12	0.49
(1,1089)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	8	0.49
(1,1089)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	16	0.49
(1,1021)	1:1610:A:ILE:HD13	1:1590:A:LEU:HD21	2	0.49
(1,996)	1:1610:A:ILE:HD11	1:1550:A:MET:HG2	16	0.49
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	20	0.49
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	14	0.49
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	2	0.49
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	19	0.49
(1,733)	1:1582:A:ARG:HG2	1:1582:A:ARG:H	11	0.49
(1,686)	1:1644:A:LEU:HD22	1:1529:A:LEU:HA	5	0.49
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	7	0.49
(1,520)	1:1541:A:ALA:HB3	1:1542:A:TYR:HD1	20	0.49
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	17	0.49
(1,431)	1:1552:A:ILE:HD11	1:1610:A:ILE:HG13	18	0.49
(1,406)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	4	0.49
(1,395)	1:1629:A:LEU:HD12	2:19:B:PHE:HD2	4	0.49
(1,389)	2:19:B:PHE:HE2	1:1626:A:LEU:HD22	2	0.49
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	14	0.49
(1,368)	1:1542:A:TYR:HE1	1:1543:A:SER:HB2	12	0.49
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	11	0.49
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	14	0.49
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG22	11	0.49
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	3	0.49
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	4	0.49
(1,309)	2:43:B:VAL:H	2:55:B:LEU:HD23	4	0.49
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA2	2	0.49
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	11	0.49
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	14	0.49
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD2	11	0.49
(1,295)	2:35:B:VAL:H	2:34:B:ARG:HG2	14	0.49
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB1	6	0.49
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	18	0.49
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	4	0.49
(1,226)	2:17:B:LEU:HD11	2:18:B:GLN:HA	11	0.49
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	10	0.49
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	19	0.49
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	2	0.49
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	5	0.49
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	13	0.49
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	10	0.49
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	16	0.49
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	4	0.49
(1,40)	1:1587:A:VAL:HG22	1:1586:A:GLN:HE21	2	0.49
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE2	18	0.49
(1,34)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	14	0.49
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	15	0.49
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	5	0.49
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	12	0.49
(1,3002)	2:42:B:ILE:HD11	2:28:B:PHE:HE2	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	19	0.48
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD1	12	0.48
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	14	0.48
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG22	20	0.48
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD12	1	0.48
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	6	0.48
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	17	0.48
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	10	0.48
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	4	0.48
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	18	0.48
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	14	0.48
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	19	0.48
(1,2473)	2:3:B:ARG:HD2	2:3:B:ARG:HB2	12	0.48
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	2	0.48
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	14	0.48
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG11	6	0.48
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD2	20	0.48
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD3	1	0.48
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	16	0.48
(1,2324)	2:64:B:ALA:HB2	2:63:B:PRO:HA	14	0.48
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	14	0.48
(1,2298)	2:55:B:LEU:HD13	2:59:B:TYR:HB2	2	0.48
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA3	2	0.48
(1,2231)	1:1567:A:PHE:HD2	1:1542:A:TYR:HD2	18	0.48
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	7	0.48
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD22	1	0.48
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	6	0.48
(1,2067)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	2	0.48
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	2	0.48
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	9	0.48
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	11	0.48
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	8	0.48
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	11	0.48
(1,1848)	1:1539:A:THR:HG23	1:1539:A:THR:H	12	0.48
(1,1848)	1:1539:A:THR:HG23	1:1539:A:THR:H	15	0.48
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	15	0.48
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	17	0.48
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	5	0.48
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	5	0.48
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	1	0.48
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	12	0.48
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	1	0.48
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	2	0.48
(1,1228)	1:1642:A:THR:HG22	1:1640:A:TRP:HE1	18	0.48
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	14	0.48
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	18	0.48
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	5	0.48
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE2	3	0.48
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	2	0.48
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	13	0.48
(1,918)	1:1570:A:THR:HG21	1:1570:A:THR:HA	4	0.48
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	14	0.48
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	5	0.48
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	10	0.48
(1,714)	1:1604:A:LEU:HD11	1:1604:A:LEU:HA	6	0.48
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD22	9	0.48
(1,622)	1:1644:A:LEU:HD11	1:1532:A:LEU:HD21	19	0.48
(1,574)	1:1547:A:VAL:HG13	1:1539:A:THR:HB	20	0.48
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	15	0.48
(1,555)	1:1547:A:VAL:HG11	1:1540:A:ALA:H	12	0.48
(1,547)	1:1642:A:THR:HG23	1:1612:A:PHE:HB2	5	0.48
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	16	0.48
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	6	0.48
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	7	0.48
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	8	0.48
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	10	0.48
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	13	0.48
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	2	0.48
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD21	13	0.48
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD11	7	0.48
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	18	0.48
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	15	0.48
(1,230)	2:55:B:LEU:HD11	2:59:B:TYR:H	19	0.48
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE2	2	0.48
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	3	0.48
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	14	0.48
(1,185)	1:1632:A:GLN:H	2:53:B:LEU:HD22	14	0.48
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	7	0.48
(1,123)	1:1523:A:THR:HG21	1:1522:A:SER:HB3	15	0.48
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	11	0.48
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	17	0.48
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	1	0.48
(1,39)	1:1548:A:VAL:HG22	1:1542:A:TYR:HE2	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:1548:A:VAL:HG21	1:1542:A:TYR:HE2	17	0.48
(1,39)	1:1548:A:VAL:HG23	1:1542:A:TYR:HE2	19	0.48
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	15	0.48
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	20	0.48
(1,2975)	2:17:B:LEU:HD12	2:17:B:LEU:HB3	20	0.47
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	11	0.47
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	5	0.47
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	12	0.47
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD13	3	0.47
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	5	0.47
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD23	10	0.47
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB1	14	0.47
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG23	18	0.47
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	8	0.47
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	7	0.47
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	7	0.47
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	19	0.47
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD13	18	0.47
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	12	0.47
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	19	0.47
(1,2451)	2:62:B:THR:HG22	2:63:B:PRO:HB3	5	0.47
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG12	20	0.47
(1,2446)	2:62:B:THR:HG23	2:62:B:THR:HA	20	0.47
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	15	0.47
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	20	0.47
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	12	0.47
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	15	0.47
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA3	10	0.47
(1,2273)	2:14:B:VAL:HG22	2:26:B:PHE:HB2	19	0.47
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	18	0.47
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	18	0.47
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	19	0.47
(1,2105)	1:1612:A:PHE:H	1:1611:A:SER:HB2	8	0.47
(1,2105)	1:1612:A:PHE:H	1:1611:A:SER:HB2	9	0.47
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG12	9	0.47
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG11	20	0.47
(1,1900)	1:1544:A:LYS:HB2	1:1545:A:SER:H	13	0.47
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD11	2	0.47
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	4	0.47
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	2	0.47
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	3	0.47
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	16	0.47
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	19	0.47
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	20	0.47
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	17	0.47
(1,1753)	1:1604:A:LEU:HD21	1:1605:A:SER:H	3	0.47
(1,1719)	1:1594:A:ASP:H	1:1594:A:ASP:HB3	3	0.47
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	14	0.47
(1,1697)	1:1644:A:LEU:HD13	1:1645:A:ALA:H	18	0.47
(1,1691)	1:1571:A:ARG:H	1:1571:A:ARG:HD3	20	0.47
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	5	0.47
(1,1586)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	17	0.47
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	9	0.47
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	17	0.47
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	4	0.47
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	8	0.47
(1,1355)	1:1621:A:THR:HG23	1:1622:A:ASN:H	12	0.47
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	14	0.47
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	10	0.47
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	11	0.47
(1,1042)	1:1609:A:VAL:HG12	1:1637:A:PHE:HB3	19	0.47
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	9	0.47
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	7	0.47
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	15	0.47
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	5	0.47
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	6	0.47
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	6	0.47
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	8	0.47
(1,733)	1:1582:A:ARG:HG2	1:1582:A:ARG:H	5	0.47
(1,714)	1:1604:A:LEU:HD22	1:1604:A:LEU:HA	2	0.47
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	9	0.47
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD12	12	0.47
(1,622)	1:1644:A:LEU:HD13	1:1532:A:LEU:HD22	11	0.47
(1,574)	1:1547:A:VAL:HG11	1:1539:A:THR:HB	6	0.47
(1,561)	1:1587:A:VAL:HG12	1:1589:A:GLN:HE22	17	0.47
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	8	0.47
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	15	0.47
(1,523)	1:1613:A:VAL:HG21	1:1641:A:HIS:HD2	1	0.47
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD13	9	0.47
(1,447)	1:1550:A:MET:HE1	1:1550:A:MET:HG2	9	0.47
(1,447)	1:1550:A:MET:HE1	1:1550:A:MET:HG2	14	0.47
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	18	0.47
(1,447)	1:1550:A:MET:HE3	1:1550:A:MET:HG2	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:1552:A:ILE:HD11	1:1610:A:ILE:HG13	19	0.47
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	20	0.47
(1,399)	2:19:B:PHE:HD2	2:16:B:THR:HG23	6	0.47
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	9	0.47
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	12	0.47
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	13	0.47
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	19	0.47
(1,285)	2:17:B:LEU:HD11	2:27:B:TYR:HD1	4	0.47
(1,248)	2:32:B:ALA:HB3	2:39:B:SER:HB3	7	0.47
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	13	0.47
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	15	0.47
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	20	0.47
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	5	0.47
(1,99)	1:1611:A:SER:HA	1:1589:A:GLN:HG3	16	0.47
(1,98)	1:1636:A:LEU:HD22	1:1606:A:TYR:HB2	10	0.47
(1,90)	1:1619:A:GLY:HA3	1:1620:A:PRO:HB3	12	0.47
(1,66)	1:1636:A:LEU:HD11	1:1638:A:PHE:HZ	16	0.47
(1,34)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	17	0.47
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	8	0.47
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	4	0.47
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	16	0.46
(1,2826)	2:59:B:TYR:H	2:58:B:THR:HG21	6	0.46
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD22	4	0.46
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	8	0.46
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	16	0.46
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD22	18	0.46
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	7	0.46
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	19	0.46
(1,2529)	2:43:B:VAL:HG22	2:44:B:GLU:HG3	20	0.46
(1,2504)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	16	0.46
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	17	0.46
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG12	2	0.46
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG11	18	0.46
(1,2445)	2:7:B:THR:HG22	2:50:B:SER:HB3	15	0.46
(1,2440)	2:17:B:LEU:HD21	2:17:B:LEU:HA	20	0.46
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	7	0.46
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	11	0.46
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	11	0.46
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	4	0.46
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	9	0.46
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA3	20	0.46
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	6	0.46
(1,1941)	1:1632:A:GLN:HG2	1:1633:A:THR:H	3	0.46
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	18	0.46
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	6	0.46
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	9	0.46
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	15	0.46
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	14	0.46
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	15	0.46
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	20	0.46
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD11	10	0.46
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	5	0.46
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	16	0.46
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	15	0.46
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	6	0.46
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	16	0.46
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	15	0.46
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	1	0.46
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	2	0.46
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG11	8	0.46
(1,1201)	1:1587:A:VAL:HG22	1:1584:A:VAL:H	4	0.46
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	1	0.46
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	11	0.46
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	8	0.46
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	9	0.46
(1,935)	1:1636:A:LEU:HD13	1:1636:A:LEU:H	12	0.46
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	12	0.46
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD21	17	0.46
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	7	0.46
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	6	0.46
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	11	0.46
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	14	0.46
(1,724)	1:1581:A:LEU:HD23	1:1588:A:LEU:HA	13	0.46
(1,715)	1:1604:A:LEU:HD11	1:1603:A:GLY:HA2	2	0.46
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD11	19	0.46
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD11	17	0.46
(1,643)	1:1604:A:LEU:HD12	1:1633:A:THR:H	19	0.46
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	1	0.46
(1,528)	1:1570:A:THR:HG21	1:1571:A:ARG:H	2	0.46
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD1	11	0.46
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	13	0.46
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD11	7	0.46
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD13	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	4	0.46
(1,447)	1:1550:A:MET:HE3	1:1550:A:MET:HG2	1	0.46
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	16	0.46
(1,442)	1:1550:A:MET:HE1	1:1640:A:TRP:HB2	18	0.46
(1,397)	1:1636:A:LEU:HD13	2:19:B:PHE:HZ	15	0.46
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD12	11	0.46
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	5	0.46
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	1	0.46
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	14	0.46
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	19	0.46
(1,311)	2:46:B:CYS:H	2:13:B:LEU:HD13	4	0.46
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	9	0.46
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	8	0.46
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	16	0.46
(1,269)	2:53:B:LEU:HD21	2:53:B:LEU:HA	19	0.46
(1,266)	2:62:B:THR:HG21	2:63:B:PRO:HG3	13	0.46
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	19	0.46
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	14	0.46
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	8	0.46
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	14	0.46
(1,185)	1:1632:A:GLN:H	2:53:B:LEU:HD21	10	0.46
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	6	0.46
(1,76)	1:1597:A:PRO:HB3	1:1596:A:SER:HB3	11	0.46
(1,32)	1:1547:A:VAL:HG22	1:1567:A:PHE:HB3	12	0.46
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	2	0.46
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	17	0.46
(1,29)	1:1609:A:VAL:HG12	1:1610:A:ILE:HB	5	0.46
(1,26)	1:1591:A:VAL:HG13	1:1607:A:LYS:HE3	12	0.46
(1,24)	1:1587:A:VAL:HG21	1:1586:A:GLN:HA	14	0.46
(1,2987)	2:42:B:ILE:HD13	2:56:B:LEU:HG	5	0.45
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	7	0.45
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	13	0.45
(1,2964)	2:20:B:VAL:HA	2:20:B:VAL:HG11	16	0.45
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	3	0.45
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	11	0.45
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE1	15	0.45
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	14	0.45
(1,2823)	2:17:B:LEU:HG	2:56:B:LEU:HB3	2	0.45
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD13	14	0.45
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB1	10	0.45
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	17	0.45
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	20	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	19	0.45
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	12	0.45
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	6	0.45
(1,2445)	2:7:B:THR:HG23	2:50:B:SER:HB3	2	0.45
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	7	0.45
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	14	0.45
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	5	0.45
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG22	2	0.45
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	4	0.45
(1,2321)	2:32:B:ALA:HB2	2:33:B:SER:HA	4	0.45
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	16	0.45
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	7	0.45
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD11	12	0.45
(1,2282)	2:42:B:ILE:HD11	2:42:B:ILE:HA	2	0.45
(1,2273)	2:14:B:VAL:HG12	2:26:B:PHE:HB2	7	0.45
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	17	0.45
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	2	0.45
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD11	9	0.45
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	14	0.45
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	7	0.45
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	3	0.45
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	15	0.45
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	2	0.45
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD12	13	0.45
(1,1848)	1:1539:A:THR:HG21	1:1539:A:THR:H	20	0.45
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG11	18	0.45
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	6	0.45
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	4	0.45
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	5	0.45
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	9	0.45
(1,1760)	1:1532:A:LEU:HD21	1:1533:A:SER:H	17	0.45
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	4	0.45
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG2	11	0.45
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	8	0.45
(1,1586)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	16	0.45
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	13	0.45
(1,1494)	1:1510:A:SER:HB2	1:1511:A:ASN:H	14	0.45
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	12	0.45
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG13	11	0.45
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG22	2	0.45
(1,1213)	1:1641:A:HIS:H	1:1641:A:HIS:HB3	12	0.45
(1,1178)	1:1609:A:VAL:HG21	1:1610:A:ILE:H	17	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1157)	1:1581:A:LEU:HD13	1:1581:A:LEU:H	2	0.45
(1,1136)	1:1590:A:LEU:HD21	1:1554:A:GLY:H	1	0.45
(1,1117)	1:1574:A:VAL:HG23	1:1608:A:SER:HA	14	0.45
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	4	0.45
(1,1056)	1:1626:A:LEU:HD11	1:1636:A:LEU:HB3	20	0.45
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	16	0.45
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	20	0.45
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	8	0.45
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	2	0.45
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	6	0.45
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	14	0.45
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	16	0.45
(1,918)	1:1570:A:THR:HG21	1:1570:A:THR:HA	18	0.45
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	2	0.45
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	3	0.45
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	15	0.45
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	20	0.45
(1,832)	1:1581:A:LEU:HD23	1:1590:A:LEU:HB2	1	0.45
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	4	0.45
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	12	0.45
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	16	0.45
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	11	0.45
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	15	0.45
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	3	0.45
(1,483)	1:1610:A:ILE:HG23	1:1590:A:LEU:HB3	7	0.45
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	2	0.45
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	3	0.45
(1,447)	1:1550:A:MET:HE2	1:1550:A:MET:HG2	11	0.45
(1,447)	1:1550:A:MET:HE1	1:1550:A:MET:HG2	12	0.45
(1,447)	1:1550:A:MET:HE1	1:1550:A:MET:HG2	17	0.45
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD1	18	0.45
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	6	0.45
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	9	0.45
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	7	0.45
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	13	0.45
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	16	0.45
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	1	0.45
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	17	0.45
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD23	13	0.45
(1,193)	1:1575:A:GLY:H	1:1606:A:TYR:HB3	7	0.45
(1,34)	1:1644:A:LEU:HD11	1:1644:A:LEU:H	16	0.45
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD12	20	0.45
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	18	0.44
(1,2992)	2:42:B:ILE:HD13	2:59:B:TYR:HE2	2	0.44
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	3	0.44
(1,2976)	2:17:B:LEU:HD22	2:17:B:LEU:HB3	14	0.44
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	1	0.44
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	6	0.44
(1,2814)	2:17:B:LEU:H	2:56:B:LEU:HD21	2	0.44
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	4	0.44
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD22	12	0.44
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD13	13	0.44
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG22	20	0.44
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	14	0.44
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	15	0.44
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD2	7	0.44
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	19	0.44
(1,2619)	2:37:B:ARG:H	2:37:B:ARG:HG2	15	0.44
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG11	9	0.44
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE1	12	0.44
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	9	0.44
(1,2472)	2:3:B:ARG:HD2	2:3:B:ARG:HB3	18	0.44
(1,2441)	2:8:B:LEU:HD13	2:8:B:LEU:HA	10	0.44
(1,2438)	2:8:B:LEU:HD23	2:8:B:LEU:HA	3	0.44
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	2	0.44
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	18	0.44
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	14	0.44
(1,2382)	2:55:B:LEU:HD23	2:51:B:CYS:HA	11	0.44
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	3	0.44
(1,2311)	2:43:B:VAL:HA	2:43:B:VAL:HG13	4	0.44
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	1	0.44
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	20	0.44
(1,2293)	2:17:B:LEU:HD13	2:56:B:LEU:HD11	11	0.44
(1,2278)	2:42:B:ILE:HD12	2:55:B:LEU:HB3	4	0.44
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD2	5	0.44
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	9	0.44
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	4	0.44
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	13	0.44
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	10	0.44
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	4	0.44
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	7	0.44
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	15	0.44
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	6	0.44
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	13	0.44
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	10	0.44
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	7	0.44
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	12	0.44
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD12	18	0.44
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	2	0.44
(1,1760)	1:1532:A:LEU:HD21	1:1533:A:SER:H	6	0.44
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	10	0.44
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	18	0.44
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	4	0.44
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	4	0.44
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	15	0.44
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG23	7	0.44
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	2	0.44
(1,1519)	1:1638:A:PHE:H	1:1609:A:VAL:HG23	2	0.44
(1,1420)	1:1588:A:LEU:H	1:1612:A:PHE:HB2	13	0.44
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG13	11	0.44
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	18	0.44
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	5	0.44
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD23	18	0.44
(1,1130)	1:1554:A:GLY:H	1:1592:A:TYR:HH	20	0.44
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	5	0.44
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	8	0.44
(1,1056)	1:1626:A:LEU:HD11	1:1636:A:LEU:HB3	19	0.44
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	12	0.44
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	11	0.44
(1,918)	1:1570:A:THR:HG21	1:1570:A:THR:HA	14	0.44
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	19	0.44
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	9	0.44
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	11	0.44
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	15	0.44
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	19	0.44
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	11	0.44
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	5	0.44
(1,745)	1:1601:A:LYS:HD3	1:1601:A:LYS:HA	15	0.44
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	4	0.44
(1,705)	1:1581:A:LEU:HD13	1:1518:A:VAL:H	1	0.44
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD13	2	0.44
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD12	3	0.44
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD11	15	0.44
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD12	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE1	20	0.44
(1,581)	1:1532:A:LEU:HD22	1:1532:A:LEU:H	8	0.44
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	1	0.44
(1,555)	1:1547:A:VAL:HG12	1:1540:A:ALA:H	20	0.44
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	13	0.44
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	2	0.44
(1,497)	1:1645:A:ALA:HB2	1:1529:A:LEU:HD12	18	0.44
(1,484)	1:1610:A:ILE:HG23	1:1610:A:ILE:HG12	6	0.44
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	12	0.44
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	3	0.44
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	14	0.44
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	15	0.44
(1,444)	1:1550:A:MET:HE1	1:1610:A:ILE:HA	6	0.44
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	6	0.44
(1,442)	1:1550:A:MET:HE2	1:1640:A:TRP:HB2	20	0.44
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD2	16	0.44
(1,423)	1:1627:A:ILE:HD13	1:1637:A:PHE:HB3	15	0.44
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	9	0.44
(1,368)	1:1542:A:TYR:HE1	1:1543:A:SER:HB2	9	0.44
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG23	16	0.44
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	11	0.44
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD2	7	0.44
(1,263)	2:56:B:LEU:HD13	2:53:B:LEU:HD22	19	0.44
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	13	0.44
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	3	0.44
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	10	0.44
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	2	0.44
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	11	0.44
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	5	0.44
(1,228)	2:55:B:LEU:HD21	2:46:B:CYS:HA	16	0.44
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	9	0.44
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	2	0.44
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG21	4	0.44
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	19	0.44
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD2	7	0.44
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	8	0.44
(1,40)	1:1587:A:VAL:HG23	1:1586:A:GLN:HE21	6	0.44
(1,40)	1:1587:A:VAL:HG21	1:1586:A:GLN:HE21	14	0.44
(1,19)	1:1618:A:ALA:HB2	1:1617:A:GLU:HB2	13	0.44
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	2	0.43
(1,3010)	2:17:B:LEU:HD22	2:56:B:LEU:HD11	8	0.43
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD11	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2987)	2:42:B:ILE:HD13	2:56:B:LEU:HG	14	0.43
(1,2976)	2:17:B:LEU:HD22	2:17:B:LEU:HB3	1	0.43
(1,2976)	2:17:B:LEU:HD21	2:17:B:LEU:HB3	2	0.43
(1,2976)	2:17:B:LEU:HD22	2:17:B:LEU:HB3	4	0.43
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	9	0.43
(1,2976)	2:17:B:LEU:HD21	2:17:B:LEU:HB3	19	0.43
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	7	0.43
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE1	8	0.43
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD23	11	0.43
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG21	8	0.43
(1,2817)	2:20:B:VAL:H	2:19:B:PHE:HE2	9	0.43
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	11	0.43
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	20	0.43
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	9	0.43
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	6	0.43
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	11	0.43
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG2	3	0.43
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	12	0.43
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	15	0.43
(1,2542)	2:50:B:SER:H	2:50:B:SER:HB3	8	0.43
(1,2507)	2:14:B:VAL:HG22	2:17:B:LEU:HD23	6	0.43
(1,2499)	2:56:B:LEU:HD12	2:20:B:VAL:HB	10	0.43
(1,2441)	2:8:B:LEU:HD11	2:8:B:LEU:HA	11	0.43
(1,2376)	2:42:B:ILE:HG22	2:28:B:PHE:HB3	13	0.43
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	10	0.43
(1,2301)	2:20:B:VAL:HG13	2:60:B:CYS:HB2	18	0.43
(1,2282)	2:42:B:ILE:HD12	2:42:B:ILE:HA	9	0.43
(1,2273)	2:14:B:VAL:HG23	2:26:B:PHE:HB2	18	0.43
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD1	14	0.43
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	11	0.43
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	9	0.43
(1,2215)	1:1644:A:LEU:HD11	1:1528:A:ASP:H	9	0.43
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	15	0.43
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	16	0.43
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	11	0.43
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	15	0.43
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD1	20	0.43
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG13	9	0.43
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	5	0.43
(1,1820)	1:1586:A:GLN:HE21	1:1586:A:GLN:HG2	18	0.43
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	1	0.43
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB2	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD11	10	0.43
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	9	0.43
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	17	0.43
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	4	0.43
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	7	0.43
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	1	0.43
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	11	0.43
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	5	0.43
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	19	0.43
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	13	0.43
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	7	0.43
(1,1679)	1:1607:A:LYS:H	1:1636:A:LEU:HD23	1	0.43
(1,1586)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	9	0.43
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	9	0.43
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	12	0.43
(1,1464)	1:1512:A:GLU:HG2	1:1512:A:GLU:H	20	0.43
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	3	0.43
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	7	0.43
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	8	0.43
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	3	0.43
(1,1178)	1:1609:A:VAL:HG22	1:1610:A:ILE:H	20	0.43
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	16	0.43
(1,1136)	1:1590:A:LEU:HD22	1:1554:A:GLY:H	16	0.43
(1,1056)	1:1626:A:LEU:HD11	1:1636:A:LEU:HB3	8	0.43
(1,1056)	1:1626:A:LEU:HD12	1:1636:A:LEU:HB3	17	0.43
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	5	0.43
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	8	0.43
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	9	0.43
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	17	0.43
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	18	0.43
(1,1040)	1:1591:A:VAL:HG23	1:1607:A:LYS:HD3	14	0.43
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	10	0.43
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HD1	12	0.43
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	3	0.43
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	14	0.43
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	7	0.43
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	4	0.43
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	6	0.43
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	10	0.43
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	14	0.43
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	15	0.43
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG21	1	0.43
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	12	0.43
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	16	0.43
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	6	0.43
(1,735)	1:1626:A:LEU:HD21	1:1542:A:TYR:HD2	18	0.43
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD12	1	0.43
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD11	3	0.43
(1,622)	1:1644:A:LEU:HD11	1:1532:A:LEU:HD22	10	0.43
(1,569)	1:1547:A:VAL:HG11	1:1539:A:THR:HG21	17	0.43
(1,563)	1:1591:A:VAL:HG13	1:1589:A:GLN:HE21	3	0.43
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	5	0.43
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	16	0.43
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	18	0.43
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	13	0.43
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	2	0.43
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	6	0.43
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	14	0.43
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	2	0.43
(1,376)	2:54:B:ALA:HB1	2:52:B:ASP:H	3	0.43
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	2	0.43
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	13	0.43
(1,364)	2:54:B:ALA:H	2:55:B:LEU:HD12	15	0.43
(1,353)	2:61:B:ALA:HB2	2:60:B:CYS:HB2	15	0.43
(1,319)	2:17:B:LEU:H	2:14:B:VAL:HG22	1	0.43
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	4	0.43
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	12	0.43
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	17	0.43
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	18	0.43
(1,293)	2:54:B:ALA:H	2:53:B:LEU:HD23	9	0.43
(1,290)	2:26:B:PHE:H	2:18:B:GLN:H	12	0.43
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	6	0.43
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	11	0.43
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	10	0.43
(1,229)	2:55:B:LEU:H	2:55:B:LEU:HD22	15	0.43
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	20	0.43
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	4	0.43
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG23	10	0.43
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	20	0.43
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	9	0.43
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	13	0.43
(1,152)	1:1592:A:TYR:H	1:1607:A:LYS:HB2	10	0.43
(1,123)	1:1523:A:THR:HG22	1:1522:A:SER:HB3	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:1610:A:ILE:HD12	1:1609:A:VAL:H	8	0.43
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	18	0.43
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	10	0.43
(1,34)	1:1644:A:LEU:HD12	1:1644:A:LEU:H	9	0.43
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	10	0.43
(1,8)	1:1610:A:ILE:HD13	1:1612:A:PHE:HZ	1	0.43
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD21	8	0.42
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	12	0.42
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG12	7	0.42
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	3	0.42
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	17	0.42
(1,2913)	2:27:B:TYR:HD1	2:27:B:TYR:HA	3	0.42
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	5	0.42
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG22	2	0.42
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG21	13	0.42
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD23	6	0.42
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	1	0.42
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	12	0.42
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	17	0.42
(1,2737)	2:56:B:LEU:H	2:56:B:LEU:HD21	11	0.42
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	13	0.42
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	2	0.42
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG21	12	0.42
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	15	0.42
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	13	0.42
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	18	0.42
(1,2500)	2:56:B:LEU:HD21	2:55:B:LEU:HD22	17	0.42
(1,2481)	2:13:B:LEU:HD11	2:14:B:VAL:HB	13	0.42
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	20	0.42
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	12	0.42
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	16	0.42
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	17	0.42
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	10	0.42
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	6	0.42
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	17	0.42
(1,2280)	2:42:B:ILE:HD12	2:41:B:GLY:HA3	14	0.42
(1,2277)	2:42:B:ILE:HD11	2:45:B:GLU:HB2	2	0.42
(1,2273)	2:14:B:VAL:HG21	2:26:B:PHE:HB2	14	0.42
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	17	0.42
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE2	2	0.42
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	12	0.42
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	18	0.42
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	20	0.42
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	3	0.42
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	12	0.42
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	13	0.42
(1,1753)	1:1604:A:LEU:HD22	1:1605:A:SER:H	12	0.42
(1,1753)	1:1604:A:LEU:HD23	1:1605:A:SER:H	19	0.42
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	5	0.42
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	14	0.42
(1,1697)	1:1644:A:LEU:HD12	1:1645:A:ALA:H	19	0.42
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG23	11	0.42
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	12	0.42
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	15	0.42
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	13	0.42
(1,1342)	1:1535:A:ARG:H	1:1534:A:GLY:HA3	3	0.42
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	4	0.42
(1,1178)	1:1609:A:VAL:HG23	1:1610:A:ILE:H	5	0.42
(1,1079)	1:1636:A:LEU:HD22	1:1626:A:LEU:HD13	14	0.42
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	14	0.42
(1,1047)	1:1609:A:VAL:HG11	1:1592:A:TYR:H	19	0.42
(1,1033)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	1	0.42
(1,1020)	1:1625:A:MET:HE1	1:1625:A:MET:HG2	15	0.42
(1,1005)	1:1532:A:LEU:HD22	1:1612:A:PHE:HZ	17	0.42
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	13	0.42
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	13	0.42
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	5	0.42
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	13	0.42
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	6	0.42
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	16	0.42
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	5	0.42
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	14	0.42
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	13	0.42
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD11	4	0.42
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	6	0.42
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD12	15	0.42
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	8	0.42
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	11	0.42
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	15	0.42
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	17	0.42
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	18	0.42
(1,574)	1:1547:A:VAL:HG11	1:1539:A:THR:HB	1	0.42
(1,574)	1:1547:A:VAL:HG13	1:1539:A:THR:HB	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:1587:A:VAL:HG13	1:1589:A:GLN:HE22	16	0.42
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	18	0.42
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	7	0.42
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	15	0.42
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	8	0.42
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	17	0.42
(1,470)	1:1572:A:ILE:HG22	1:1596:A:SER:HA	5	0.42
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	7	0.42
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	11	0.42
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	13	0.42
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	19	0.42
(1,442)	1:1550:A:MET:HE2	1:1640:A:TRP:HB2	2	0.42
(1,396)	1:1542:A:TYR:HD2	2:19:B:PHE:HD1	20	0.42
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	19	0.42
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	5	0.42
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	1	0.42
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	1	0.42
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	8	0.42
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	2	0.42
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	10	0.42
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	3	0.42
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	19	0.42
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	14	0.42
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	13	0.42
(1,32)	1:1547:A:VAL:HG21	1:1567:A:PHE:HB3	1	0.42
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	4	0.42
(1,30)	1:1587:A:VAL:HG21	1:1585:A:ASP:H	7	0.42
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	18	0.41
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	10	0.41
(1,2976)	2:17:B:LEU:HD22	2:17:B:LEU:HB3	11	0.41
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD21	4	0.41
(1,2913)	2:27:B:TYR:HD1	2:27:B:TYR:HA	19	0.41
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	17	0.41
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD23	19	0.41
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD12	20	0.41
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	16	0.41
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	8	0.41
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD22	12	0.41
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG22	16	0.41
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	3	0.41
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	11	0.41
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	17	0.41
(1,2504)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	9	0.41
(1,2459)	2:56:B:LEU:HD22	2:53:B:LEU:HB2	2	0.41
(1,2440)	2:17:B:LEU:HD21	2:17:B:LEU:HA	5	0.41
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	1	0.41
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	9	0.41
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	13	0.41
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	15	0.41
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	18	0.41
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	9	0.41
(1,2322)	2:32:B:ALA:HB1	2:33:B:SER:HB3	12	0.41
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	8	0.41
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	12	0.41
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	10	0.41
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	4	0.41
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	7	0.41
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	10	0.41
(1,2215)	1:1644:A:LEU:HD11	1:1528:A:ASP:H	13	0.41
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	19	0.41
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	3	0.41
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	12	0.41
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	2	0.41
(1,1953)	1:1595:A:GLY:H	1:1605:A:SER:HB3	4	0.41
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	11	0.41
(1,1837)	1:1618:A:ALA:HB1	1:1622:A:ASN:HD22	1	0.41
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	3	0.41
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	5	0.41
(1,1789)	1:1577:A:ALA:HB2	1:1578:A:ASN:H	6	0.41
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	19	0.41
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	17	0.41
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	13	0.41
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	17	0.41
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	11	0.41
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD11	12	0.41
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	2	0.41
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	10	0.41
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	14	0.41
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	15	0.41
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	6	0.41
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	5	0.41
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	14	0.41
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	7	0.41
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	6	0.41
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	11	0.41
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	15	0.41
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	17	0.41
(1,1249)	1:1529:A:LEU:HD22	1:1529:A:LEU:H	14	0.41
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG23	6	0.41
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	14	0.41
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	16	0.41
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	18	0.41
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG11	4	0.41
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	6	0.41
(1,1056)	1:1626:A:LEU:HD13	1:1636:A:LEU:HB3	7	0.41
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	1	0.41
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	7	0.41
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	13	0.41
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	7	0.41
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	9	0.41
(1,1033)	1:1645:A:ALA:HB1	1:1614:A:CYS:HB3	9	0.41
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HZ	11	0.41
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	15	0.41
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	2	0.41
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	4	0.41
(1,933)	1:1626:A:LEU:HD12	1:1636:A:LEU:HG	5	0.41
(1,918)	1:1570:A:THR:HG21	1:1570:A:THR:HA	6	0.41
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	3	0.41
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	12	0.41
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	1	0.41
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	20	0.41
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG23	20	0.41
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	2	0.41
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	6	0.41
(1,705)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	5	0.41
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	19	0.41
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD13	20	0.41
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD21	4	0.41
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	15	0.41
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	4	0.41
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	9	0.41
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	11	0.41
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	13	0.41
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:1572:A:ILE:HG22	1:1596:A:SER:HA	6	0.41
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	11	0.41
(1,408)	1:1545:A:SER:H	2:18:B:GLN:HG2	10	0.41
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	12	0.41
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	5	0.41
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	16	0.41
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	2	0.41
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	16	0.41
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	5	0.41
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	12	0.41
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	6	0.41
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	1	0.41
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	9	0.41
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	18	0.41
(1,230)	2:55:B:LEU:HD13	2:59:B:TYR:H	14	0.41
(1,125)	1:1591:A:VAL:HG22	1:1582:A:ARG:HD2	4	0.41
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	13	0.41
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	6	0.41
(1,53)	1:1588:A:LEU:HD11	1:1583:A:TYR:H	9	0.41
(1,28)	1:1609:A:VAL:HG22	1:1607:A:LYS:HB3	15	0.41
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	7	0.41
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	15	0.4
(1,2932)	2:65:B:LYS:H	2:65:B:LYS:HB3	20	0.4
(1,2826)	2:59:B:TYR:H	2:58:B:THR:HG22	2	0.4
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	20	0.4
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	9	0.4
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	8	0.4
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD22	4	0.4
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	6	0.4
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	19	0.4
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG2	18	0.4
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	6	0.4
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	9	0.4
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG21	7	0.4
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	1	0.4
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	10	0.4
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG2	19	0.4
(1,2482)	2:13:B:LEU:HD12	2:12:B:GLU:HB3	18	0.4
(1,2482)	2:13:B:LEU:HD11	2:12:B:GLU:HB3	20	0.4
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	19	0.4
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	12	0.4
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	3	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	4	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	5	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	7	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	11	0.4
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	19	0.4
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	5	0.4
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG21	5	0.4
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	18	0.4
(1,2293)	2:17:B:LEU:HD13	2:56:B:LEU:HD11	8	0.4
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	20	0.4
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG23	2	0.4
(1,2246)	1:1583:A:TYR:HE1	1:1522:A:SER:H	5	0.4
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	7	0.4
(1,2215)	1:1644:A:LEU:HD12	1:1528:A:ASP:H	6	0.4
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	6	0.4
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	15	0.4
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	7	0.4
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	12	0.4
(1,1895)	1:1545:A:SER:H	1:1543:A:SER:HB2	20	0.4
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	4	0.4
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	17	0.4
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	18	0.4
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	8	0.4
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	10	0.4
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	18	0.4
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	18	0.4
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	2	0.4
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	6	0.4
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	19	0.4
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	2	0.4
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	3	0.4
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	20	0.4
(1,1494)	1:1510:A:SER:HB3	1:1511:A:ASN:H	15	0.4
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB3	8	0.4
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	11	0.4
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	16	0.4
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	4	0.4
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	6	0.4
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	8	0.4
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	1	0.4
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	6	0.4
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	9	0.4
(1,1300)	1:1563:A:VAL:H	1:1563:A:VAL:HG12	10	0.4
(1,1228)	1:1642:A:THR:HG22	1:1640:A:TRP:HE1	19	0.4
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	9	0.4
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	12	0.4
(1,1174)	1:1591:A:VAL:HG12	1:1592:A:TYR:H	13	0.4
(1,1157)	1:1581:A:LEU:HD13	1:1581:A:LEU:H	3	0.4
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	19	0.4
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	6	0.4
(1,1110)	1:1583:A:TYR:HD2	1:1584:A:VAL:HG21	20	0.4
(1,1094)	1:1588:A:LEU:HD12	1:1581:A:LEU:HG	1	0.4
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	11	0.4
(1,1056)	1:1626:A:LEU:HD13	1:1636:A:LEU:HB3	2	0.4
(1,1056)	1:1626:A:LEU:HD12	1:1636:A:LEU:HB3	9	0.4
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	10	0.4
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	5	0.4
(1,1020)	1:1625:A:MET:HE1	1:1625:A:MET:HG2	2	0.4
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	9	0.4
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	19	0.4
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	12	0.4
(1,996)	1:1610:A:ILE:HD11	1:1550:A:MET:HG2	17	0.4
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	16	0.4
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	14	0.4
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	17	0.4
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG12	16	0.4
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	17	0.4
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	8	0.4
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	5	0.4
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	8	0.4
(1,782)	1:1569:A:GLN:HG2	1:1570:A:THR:H	5	0.4
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	16	0.4
(1,637)	1:1518:A:VAL:HG13	1:1581:A:LEU:HD22	14	0.4
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	8	0.4
(1,584)	1:1540:A:ALA:HB1	1:1638:A:PHE:HD1	17	0.4
(1,538)	1:1570:A:THR:HG23	1:1569:A:GLN:HB3	20	0.4
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	10	0.4
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	17	0.4
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	15	0.4
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	9	0.4
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	10	0.4
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD2	18	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:1577:A:ALA:HB3	1:1565:A:ALA:H	2	0.4
(1,484)	1:1610:A:ILE:HG21	1:1610:A:ILE:HG12	1	0.4
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	5	0.4
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	10	0.4
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	3	0.4
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	10	0.4
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	12	0.4
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	15	0.4
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	20	0.4
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	12	0.4
(1,363)	1:1632:A:GLN:H	1:1629:A:LEU:HD13	3	0.4
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	19	0.4
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	3	0.4
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	11	0.4
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	4	0.4
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	8	0.4
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	18	0.4
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	2	0.4
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	1	0.4
(1,226)	2:17:B:LEU:HD13	2:57:B:GLU:HA	4	0.4
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	8	0.4
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	3	0.4
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	16	0.4
(1,82)	1:1589:A:GLN:HG2	1:1590:A:LEU:HA	16	0.4
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	10	0.4
(1,32)	1:1547:A:VAL:HG22	1:1549:A:TYR:HB3	14	0.4
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	5	0.4
(1,17)	1:1577:A:ALA:HB2	1:1553:A:CYS:H	20	0.4
(1,14)	1:1552:A:ILE:HG22	1:1529:A:LEU:HD11	18	0.4
(1,11)	1:1625:A:MET:HE2	1:1624:A:PRO:HA	7	0.4
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	9	0.39
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	19	0.39
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	4	0.39
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD21	7	0.39
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	1	0.39
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	18	0.39
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	16	0.39
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	3	0.39
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	14	0.39
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	15	0.39
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	9	0.39
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE1	18	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	10	0.39
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	10	0.39
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	11	0.39
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	8	0.39
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	8	0.39
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	9	0.39
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	12	0.39
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	17	0.39
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	6	0.39
(1,2376)	2:42:B:ILE:HG23	2:28:B:PHE:HB3	10	0.39
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	19	0.39
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	2	0.39
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG22	11	0.39
(1,2273)	2:14:B:VAL:HG12	2:26:B:PHE:HB2	11	0.39
(1,2259)	2:42:B:ILE:HG22	2:28:B:PHE:HD1	11	0.39
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	2	0.39
(1,2162)	1:1539:A:THR:HG21	1:1547:A:VAL:H	12	0.39
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	20	0.39
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	2	0.39
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	14	0.39
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG11	11	0.39
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	18	0.39
(1,1895)	1:1545:A:SER:H	1:1543:A:SER:HB2	14	0.39
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	18	0.39
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	16	0.39
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	12	0.39
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	19	0.39
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	3	0.39
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG11	3	0.39
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	11	0.39
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	1	0.39
(1,1564)	1:1531:A:SER:HB3	1:1531:A:SER:H	17	0.39
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	13	0.39
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	19	0.39
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	14	0.39
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	13	0.39
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	4	0.39
(1,1174)	1:1591:A:VAL:HG12	1:1592:A:TYR:H	7	0.39
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	17	0.39
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	3	0.39
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	8	0.39
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:1518:A:VAL:HG21	1:1582:A:ARG:HA	14	0.39
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	3	0.39
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	7	0.39
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	8	0.39
(1,1020)	1:1625:A:MET:HE1	1:1625:A:MET:HG2	17	0.39
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	1	0.39
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	2	0.39
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	7	0.39
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG22	8	0.39
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	13	0.39
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	10	0.39
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	12	0.39
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	17	0.39
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	20	0.39
(1,933)	1:1626:A:LEU:HD13	1:1636:A:LEU:HG	2	0.39
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	20	0.39
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	4	0.39
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	14	0.39
(1,724)	1:1581:A:LEU:HD21	1:1588:A:LEU:HA	7	0.39
(1,724)	1:1581:A:LEU:HD21	1:1588:A:LEU:HA	9	0.39
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD11	12	0.39
(1,623)	1:1588:A:LEU:HD23	1:1589:A:GLN:H	9	0.39
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	20	0.39
(1,614)	1:1626:A:LEU:HD21	1:1636:A:LEU:HB2	19	0.39
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	6	0.39
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	12	0.39
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	15	0.39
(1,452)	1:1572:A:ILE:HD11	1:1572:A:ILE:HA	16	0.39
(1,387)	1:1572:A:ILE:HD11	2:16:B:THR:H	9	0.39
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	9	0.39
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG22	18	0.39
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	3	0.39
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	20	0.39
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	4	0.39
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	6	0.39
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	8	0.39
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	4	0.39
(1,226)	2:17:B:LEU:HD13	2:18:B:GLN:HA	12	0.39
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	5	0.39
(1,204)	1:1610:A:ILE:HG22	1:1639:A:SER:H	8	0.39
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD3	12	0.39
(1,97)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:1547:A:VAL:HG22	1:1567:A:PHE:HB3	3	0.39
(1,29)	1:1609:A:VAL:HG11	1:1610:A:ILE:HB	6	0.39
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	9	0.38
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	12	0.38
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE2	8	0.38
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	13	0.38
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	16	0.38
(1,2976)	2:17:B:LEU:HD23	2:17:B:LEU:HB3	18	0.38
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD2	4	0.38
(1,2861)	2:20:B:VAL:HG23	2:19:B:PHE:HD2	3	0.38
(1,2848)	2:55:B:LEU:HD11	2:59:B:TYR:HE2	3	0.38
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	15	0.38
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG21	15	0.38
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD23	16	0.38
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD13	2	0.38
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	10	0.38
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD2	19	0.38
(1,2699)	2:3:B:ARG:H	2:3:B:ARG:HB3	17	0.38
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	18	0.38
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	12	0.38
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	5	0.38
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	18	0.38
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	8	0.38
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	18	0.38
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	14	0.38
(1,2504)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	4	0.38
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	3	0.38
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	9	0.38
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	17	0.38
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	18	0.38
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	8	0.38
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	13	0.38
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	1	0.38
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	2	0.38
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	6	0.38
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	13	0.38
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	12	0.38
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	13	0.38
(1,2322)	2:32:B:ALA:HB2	2:33:B:SER:HB3	8	0.38
(1,2315)	2:43:B:VAL:HG22	2:40:B:ARG:HD3	4	0.38
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	20	0.38
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	14	0.38
(1,2295)	2:17:B:LEU:HD23	2:56:B:LEU:HA	20	0.38
(1,2232)	1:1567:A:PHE:HD1	1:1542:A:TYR:HE1	11	0.38
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	4	0.38
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	19	0.38
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	15	0.38
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD1	11	0.38
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	3	0.38
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	5	0.38
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	16	0.38
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG13	6	0.38
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG12	15	0.38
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	10	0.38
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	12	0.38
(1,1848)	1:1539:A:THR:HG23	1:1539:A:THR:H	1	0.38
(1,1837)	1:1618:A:ALA:HB1	1:1622:A:ASN:HD22	15	0.38
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	12	0.38
(1,1789)	1:1577:A:ALA:HB1	1:1578:A:ASN:H	4	0.38
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD12	14	0.38
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	4	0.38
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	19	0.38
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	15	0.38
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	20	0.38
(1,1639)	1:1646:A:CYS:HB3	1:1646:A:CYS:H	13	0.38
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	9	0.38
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	18	0.38
(1,1586)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	13	0.38
(1,1496)	1:1574:A:VAL:H	1:1574:A:VAL:HG11	7	0.38
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	15	0.38
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	20	0.38
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	15	0.38
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	7	0.38
(1,1373)	1:1572:A:ILE:HG22	1:1572:A:ILE:H	8	0.38
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	18	0.38
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	20	0.38
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	19	0.38
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	19	0.38
(1,1330)	1:1569:A:GLN:H	1:1568:A:GLY:HA2	15	0.38
(1,1228)	1:1642:A:THR:HG23	1:1640:A:TRP:HE1	2	0.38
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	13	0.38
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	18	0.38
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	10	0.38
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	18	0.38
(1,1089)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	1	0.38
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	9	0.38
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	14	0.38
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	15	0.38
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	9	0.38
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	10	0.38
(1,1020)	1:1625:A:MET:HE1	1:1625:A:MET:HG2	12	0.38
(1,1020)	1:1625:A:MET:HE3	1:1625:A:MET:HG2	13	0.38
(1,1020)	1:1625:A:MET:HE2	1:1625:A:MET:HG2	20	0.38
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	16	0.38
(1,991)	1:1618:A:ALA:HB2	1:1617:A:GLU:HA	8	0.38
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	16	0.38
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	5	0.38
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	3	0.38
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	15	0.38
(1,962)	1:1526:A:LEU:HD21	1:1526:A:LEU:HB3	18	0.38
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	4	0.38
(1,933)	1:1626:A:LEU:HD13	1:1636:A:LEU:HG	7	0.38
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	12	0.38
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	13	0.38
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	4	0.38
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	4	0.38
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	2	0.38
(1,697)	1:1644:A:LEU:HD12	1:1529:A:LEU:HD12	6	0.38
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	19	0.38
(1,659)	1:1526:A:LEU:HD22	1:1527:A:PHE:HA	8	0.38
(1,574)	1:1547:A:VAL:HG12	1:1539:A:THR:HB	12	0.38
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	2	0.38
(1,534)	1:1523:A:THR:HG22	1:1523:A:THR:HA	3	0.38
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	14	0.38
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	19	0.38
(1,534)	1:1523:A:THR:HG23	1:1523:A:THR:HA	20	0.38
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	18	0.38
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	5	0.38
(1,424)	1:1552:A:ILE:HD11	1:1592:A:TYR:HH	9	0.38
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	17	0.38
(1,411)	1:1602:A:SER:H	2:52:B:ASP:HA	4	0.38
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD11	5	0.38
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	20	0.38
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	2:55:B:LEU:HD11	2:56:B:LEU:H	4	0.38
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	8	0.38
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	15	0.38
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	5	0.38
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	17	0.38
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	9	0.38
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD2	12	0.38
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	19	0.38
(1,275)	2:13:B:LEU:HD21	2:8:B:LEU:HA	14	0.38
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	18	0.38
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	20	0.38
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	1	0.38
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	19	0.38
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	13	0.38
(1,97)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	4	0.38
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD13	9	0.38
(1,74)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	11	0.38
(1,34)	1:1644:A:LEU:HD13	1:1644:A:LEU:H	13	0.38
(1,21)	1:1645:A:ALA:HB3	1:1612:A:PHE:HA	11	0.38
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	17	0.38
(1,10)	1:1550:A:MET:HE1	1:1549:A:TYR:HA	5	0.38
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	20	0.37
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	8	0.37
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	2	0.37
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD22	2	0.37
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD1	14	0.37
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	17	0.37
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG21	5	0.37
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG21	8	0.37
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	13	0.37
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD22	16	0.37
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB2	11	0.37
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	12	0.37
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG3	14	0.37
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	14	0.37
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	3	0.37
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	4	0.37
(1,2431)	2:4:B:PRO:HB2	2:4:B:PRO:HD3	14	0.37
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	10	0.37
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	20	0.37
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	16	0.37
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	4	0.37
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	4	0.37
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	7	0.37
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	4	0.37
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD21	4	0.37
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD22	19	0.37
(1,1837)	1:1618:A:ALA:HB2	1:1622:A:ASN:HD22	12	0.37
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	16	0.37
(1,1753)	1:1604:A:LEU:HD22	1:1605:A:SER:H	4	0.37
(1,1718)	1:1579:A:LYS:H	1:1578:A:ASN:HB3	7	0.37
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG23	1	0.37
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	18	0.37
(1,1494)	1:1510:A:SER:HB3	1:1511:A:ASN:H	4	0.37
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	18	0.37
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	9	0.37
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	2	0.37
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	3	0.37
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	14	0.37
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	18	0.37
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	8	0.37
(1,1323)	1:1563:A:VAL:HG22	1:1577:A:ALA:H	18	0.37
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG22	14	0.37
(1,1174)	1:1591:A:VAL:HG12	1:1592:A:TYR:H	10	0.37
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	14	0.37
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	11	0.37
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	5	0.37
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	4	0.37
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	1	0.37
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	17	0.37
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	7	0.37
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	1	0.37
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	3	0.37
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	6	0.37
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	3	0.37
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	10	0.37
(1,1045)	1:1587:A:VAL:HG12	1:1587:A:VAL:H	16	0.37
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	17	0.37
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	17	0.37
(1,1020)	1:1625:A:MET:HE3	1:1625:A:MET:HG2	14	0.37
(1,1019)	1:1625:A:MET:HE2	1:1625:A:MET:HG3	18	0.37
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	5	0.37
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	19	0.37
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	4	0.37
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	8	0.37
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	11	0.37
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	14	0.37
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	10	0.37
(1,933)	1:1626:A:LEU:HD12	1:1636:A:LEU:HG	17	0.37
(1,832)	1:1581:A:LEU:HD21	1:1590:A:LEU:HB2	14	0.37
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	11	0.37
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	19	0.37
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	10	0.37
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	8	0.37
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	15	0.37
(1,725)	1:1581:A:LEU:HD23	1:1517:A:GLN:HA	13	0.37
(1,724)	1:1581:A:LEU:HD23	1:1588:A:LEU:HA	20	0.37
(1,711)	1:1604:A:LEU:HD22	1:1605:A:SER:H	16	0.37
(1,693)	1:1590:A:LEU:HD21	1:1592:A:TYR:HA	8	0.37
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	5	0.37
(1,637)	1:1518:A:VAL:HG11	1:1581:A:LEU:HD22	11	0.37
(1,636)	1:1588:A:LEU:HD23	1:1529:A:LEU:HD11	13	0.37
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	6	0.37
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	19	0.37
(1,614)	1:1626:A:LEU:HD21	1:1636:A:LEU:HB2	20	0.37
(1,599)	1:1587:A:VAL:HG12	1:1611:A:SER:HB2	10	0.37
(1,542)	1:1613:A:VAL:HG11	1:1641:A:HIS:HA	12	0.37
(1,536)	1:1609:A:VAL:HG23	1:1607:A:LYS:HE3	3	0.37
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	10	0.37
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	13	0.37
(1,483)	1:1610:A:ILE:HG21	1:1590:A:LEU:HB3	20	0.37
(1,470)	1:1572:A:ILE:HG21	1:1596:A:SER:HA	4	0.37
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	7	0.37
(1,411)	1:1602:A:SER:H	2:52:B:ASP:HA	16	0.37
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	7	0.37
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	13	0.37
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD11	8	0.37
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	20	0.37
(1,329)	2:59:B:TYR:HD1	2:42:B:ILE:H	17	0.37
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	20	0.37
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	11	0.37
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	16	0.37
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	7	0.37
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	2:26:B:PHE:H	2:24:B:ARG:H	13	0.37
(1,245)	2:42:B:ILE:HD11	2:43:B:VAL:HA	11	0.37
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	10	0.37
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	7	0.37
(1,203)	1:1598:A:CYS:H	1:1603:A:GLY:HA2	9	0.37
(1,189)	1:1635:A:THR:H	1:1633:A:THR:HG22	4	0.37
(1,125)	1:1591:A:VAL:HG23	1:1582:A:ARG:HD2	2	0.37
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	1	0.37
(1,84)	1:1589:A:GLN:HG2	1:1582:A:ARG:HD2	6	0.37
(1,62)	1:1588:A:LEU:HD13	1:1645:A:ALA:HA	15	0.37
(1,32)	1:1547:A:VAL:HG21	1:1549:A:TYR:HB3	18	0.37
(1,11)	1:1625:A:MET:HE3	1:1624:A:PRO:HA	20	0.37
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	10	0.37
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	10	0.36
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	8	0.36
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	19	0.36
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	5	0.36
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG22	19	0.36
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	1	0.36
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	5	0.36
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	5	0.36
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	13	0.36
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	18	0.36
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	11	0.36
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	1	0.36
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	3	0.36
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	9	0.36
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	5	0.36
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	4	0.36
(1,2482)	2:13:B:LEU:HD11	2:12:B:GLU:HB3	17	0.36
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	8	0.36
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	16	0.36
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	15	0.36
(1,2419)	2:63:B:PRO:HD3	2:63:B:PRO:HG3	18	0.36
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	2	0.36
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	14	0.36
(1,2323)	2:32:B:ALA:HB2	2:33:B:SER:HB2	16	0.36
(1,2321)	2:32:B:ALA:HB2	2:33:B:SER:HA	3	0.36
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG21	2	0.36
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	15	0.36
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE2	2	0.36
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD12	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	6	0.36
(1,2273)	2:14:B:VAL:HG23	2:26:B:PHE:HB2	10	0.36
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG21	12	0.36
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	13	0.36
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	20	0.36
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	11	0.36
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	3	0.36
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	16	0.36
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	10	0.36
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	20	0.36
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	18	0.36
(1,1782)	1:1517:A:GLN:H	1:1515:A:ASP:HB3	8	0.36
(1,1760)	1:1532:A:LEU:HD23	1:1533:A:SER:H	11	0.36
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	19	0.36
(1,1717)	1:1646:A:CYS:HB2	1:1646:A:CYS:H	12	0.36
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	9	0.36
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	3	0.36
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	19	0.36
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	3	0.36
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	5	0.36
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	13	0.36
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	10	0.36
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	11	0.36
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	2	0.36
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	11	0.36
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	3	0.36
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	14	0.36
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	15	0.36
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	11	0.36
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	6	0.36
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	14	0.36
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	19	0.36
(1,1060)	1:1529:A:LEU:HD22	1:1581:A:LEU:HG	1	0.36
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	4	0.36
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	6	0.36
(1,1057)	1:1626:A:LEU:HD22	1:1628:A:SER:H	15	0.36
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	3	0.36
(1,1044)	1:1518:A:VAL:HG21	1:1582:A:ARG:HA	8	0.36
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	15	0.36
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	18	0.36
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	13	0.36
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:1625:A:MET:HE3	1:1625:A:MET:HG2	6	0.36
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	4	0.36
(1,996)	1:1610:A:ILE:HD11	1:1550:A:MET:HG2	15	0.36
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	17	0.36
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	7	0.36
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	5	0.36
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	6	0.36
(1,962)	1:1526:A:LEU:HD21	1:1526:A:LEU:HB3	19	0.36
(1,933)	1:1626:A:LEU:HD12	1:1636:A:LEU:HG	9	0.36
(1,933)	1:1626:A:LEU:HD11	1:1636:A:LEU:HG	19	0.36
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE1	1	0.36
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	8	0.36
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	10	0.36
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	2	0.36
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	8	0.36
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	8	0.36
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	10	0.36
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG21	17	0.36
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	12	0.36
(1,680)	1:1529:A:LEU:HD13	1:1588:A:LEU:HD13	16	0.36
(1,680)	1:1529:A:LEU:HD12	1:1588:A:LEU:HD12	18	0.36
(1,668)	1:1635:A:THR:HG22	1:1607:A:LYS:HG3	8	0.36
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	10	0.36
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	20	0.36
(1,650)	1:1590:A:LEU:HD22	1:1581:A:LEU:H	6	0.36
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	5	0.36
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	3	0.36
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	9	0.36
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG23	7	0.36
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	13	0.36
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	1	0.36
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	15	0.36
(1,495)	1:1572:A:ILE:HG23	1:1606:A:TYR:HD2	11	0.36
(1,493)	1:1577:A:ALA:HB3	1:1565:A:ALA:H	7	0.36
(1,483)	1:1610:A:ILE:HG23	1:1590:A:LEU:HB3	14	0.36
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	5	0.36
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	12	0.36
(1,451)	1:1550:A:MET:HE1	1:1610:A:ILE:HG13	18	0.36
(1,431)	1:1552:A:ILE:HD12	1:1610:A:ILE:HG13	17	0.36
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD11	5	0.36
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	8	0.36
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD11	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	2:18:B:GLN:HE21	2:14:B:VAL:HG12	19	0.36
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	10	0.36
(1,354)	2:38:B:ARG:HE	2:59:B:TYR:HE2	19	0.36
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	4	0.36
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	5	0.36
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD22	6	0.36
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	11	0.36
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG2	6	0.36
(1,245)	2:42:B:ILE:HD13	2:14:B:VAL:HA	16	0.36
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	1	0.36
(1,228)	2:55:B:LEU:HD21	2:46:B:CYS:HA	4	0.36
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	6	0.36
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	7	0.36
(1,228)	2:55:B:LEU:HD12	2:46:B:CYS:HA	15	0.36
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	6	0.36
(1,181)	1:1616:A:PRO:HB3	1:1617:A:GLU:H	5	0.36
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	7	0.36
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	10	0.36
(1,70)	1:1550:A:MET:HG3	1:1540:A:ALA:HB2	4	0.36
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	14	0.36
(1,32)	1:1547:A:VAL:HG21	1:1567:A:PHE:HB3	17	0.36
(1,29)	1:1609:A:VAL:HG13	1:1610:A:ILE:HB	1	0.36
(1,26)	1:1591:A:VAL:HG13	1:1593:A:LYS:HE3	5	0.36
(1,17)	1:1577:A:ALA:HB1	1:1553:A:CYS:H	7	0.36
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	14	0.36
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	14	0.35
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	14	0.35
(1,3009)	2:56:B:LEU:HD23	2:17:B:LEU:HD23	13	0.35
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD11	15	0.35
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG12	11	0.35
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	13	0.35
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	12	0.35
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	19	0.35
(1,2817)	2:20:B:VAL:H	2:19:B:PHE:HE2	13	0.35
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG13	1	0.35
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD11	6	0.35
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	3	0.35
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	15	0.35
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	19	0.35
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	20	0.35
(1,2525)	2:58:B:THR:HG23	2:59:B:TYR:HE2	20	0.35
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2515)	2:55:B:LEU:HD21	2:46:B:CYS:HA	16	0.35
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	19	0.35
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	1	0.35
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	2	0.35
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	1	0.35
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	4	0.35
(1,2451)	2:62:B:THR:HG23	2:63:B:PRO:HB3	1	0.35
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	13	0.35
(1,2376)	2:42:B:ILE:HG22	2:28:B:PHE:HB3	18	0.35
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	20	0.35
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	5	0.35
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	14	0.35
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG21	19	0.35
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	20	0.35
(1,2273)	2:14:B:VAL:HG22	2:26:B:PHE:HB2	9	0.35
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	7	0.35
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	11	0.35
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE1	12	0.35
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG22	7	0.35
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	17	0.35
(1,2105)	1:1612:A:PHE:H	1:1611:A:SER:HB2	7	0.35
(1,2067)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	7	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	9	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	10	0.35
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG11	19	0.35
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	15	0.35
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	1	0.35
(1,1757)	1:1533:A:SER:HB3	1:1533:A:SER:H	14	0.35
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	3	0.35
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	16	0.35
(1,1718)	1:1579:A:LYS:H	1:1578:A:ASN:HB3	14	0.35
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	6	0.35
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	14	0.35
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	17	0.35
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	19	0.35
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	13	0.35
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	15	0.35
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	7	0.35
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	9	0.35
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	11	0.35
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	13	0.35
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG22	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	13	0.35
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	13	0.35
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	15	0.35
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	8	0.35
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	7	0.35
(1,1114)	1:1583:A:TYR:HE1	1:1585:A:ASP:HA	7	0.35
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	6	0.35
(1,1045)	1:1587:A:VAL:HG12	1:1587:A:VAL:H	8	0.35
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	1	0.35
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	2	0.35
(1,1044)	1:1518:A:VAL:HG21	1:1582:A:ARG:HA	4	0.35
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	10	0.35
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	16	0.35
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	19	0.35
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	20	0.35
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	15	0.35
(1,1034)	1:1518:A:VAL:HG23	1:1518:A:VAL:HA	4	0.35
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	7	0.35
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	11	0.35
(1,1034)	1:1518:A:VAL:HG23	1:1518:A:VAL:HA	14	0.35
(1,1019)	1:1625:A:MET:HE1	1:1625:A:MET:HG3	5	0.35
(1,962)	1:1526:A:LEU:HD22	1:1526:A:LEU:HB3	1	0.35
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	16	0.35
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	1	0.35
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	3	0.35
(1,691)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	15	0.35
(1,664)	1:1607:A:LYS:HG3	1:1607:A:LYS:HE3	20	0.35
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	1	0.35
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	6	0.35
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	9	0.35
(1,547)	1:1642:A:THR:HG22	1:1612:A:PHE:HB2	7	0.35
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE2	18	0.35
(1,523)	1:1613:A:VAL:HG22	1:1641:A:HIS:HD2	7	0.35
(1,523)	1:1613:A:VAL:HG23	1:1641:A:HIS:HD2	9	0.35
(1,512)	1:1645:A:ALA:HB2	1:1614:A:CYS:H	5	0.35
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	16	0.35
(1,480)	1:1627:A:ILE:HG22	1:1626:A:LEU:HD11	2	0.35
(1,452)	1:1572:A:ILE:HD13	1:1572:A:ILE:HA	8	0.35
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	4	0.35
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	19	0.35
(1,411)	1:1602:A:SER:H	1:1600:A:SER:HA	11	0.35
(1,391)	2:19:B:PHE:HE1	1:1548:A:VAL:HG23	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	2:54:B:ALA:HB2	2:52:B:ASP:H	4	0.35
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	5	0.35
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	17	0.35
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	6	0.35
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	20	0.35
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA2	11	0.35
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	8	0.35
(1,269)	2:53:B:LEU:HD21	2:53:B:LEU:HA	17	0.35
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	7	0.35
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	20	0.35
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	1	0.35
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	7	0.35
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	6	0.35
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	16	0.35
(1,69)	1:1617:A:GLU:HB2	1:1618:A:ALA:H	7	0.35
(1,32)	1:1547:A:VAL:HG22	1:1549:A:TYR:HB3	13	0.35
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG12	4	0.35
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	14	0.35
(1,3019)	2:18:B:GLN:HG3	1:1545:A:SER:HB3	14	0.34
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	18	0.34
(1,3013)	1:1629:A:LEU:HD12	2:19:B:PHE:HZ	19	0.34
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	19	0.34
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD11	7	0.34
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD11	9	0.34
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	19	0.34
(1,2987)	2:42:B:ILE:HD11	2:56:B:LEU:HG	18	0.34
(1,2960)	2:42:B:ILE:HG12	2:28:B:PHE:HD1	9	0.34
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	4	0.34
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	18	0.34
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	4	0.34
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	13	0.34
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD21	10	0.34
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	12	0.34
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	20	0.34
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG2	6	0.34
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	5	0.34
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	11	0.34
(1,2463)	2:56:B:LEU:HD22	2:55:B:LEU:H	4	0.34
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	5	0.34
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	20	0.34
(1,2445)	2:7:B:THR:HG21	2:50:B:SER:HB3	19	0.34
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	3	0.34
(1,2378)	2:42:B:ILE:HG22	2:59:B:TYR:HB3	6	0.34
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	20	0.34
(1,2324)	2:64:B:ALA:HB3	2:63:B:PRO:HA	6	0.34
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG21	3	0.34
(1,2304)	2:21:B:CYS:H	2:20:B:VAL:HG23	7	0.34
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	12	0.34
(1,2289)	2:42:B:ILE:HD13	2:55:B:LEU:HD11	2	0.34
(1,2286)	2:42:B:ILE:HD11	2:28:B:PHE:HD2	20	0.34
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	8	0.34
(1,2251)	2:55:B:LEU:HD11	2:59:B:TYR:HE2	13	0.34
(1,2215)	1:1644:A:LEU:HD11	1:1528:A:ASP:H	1	0.34
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	17	0.34
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	8	0.34
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	20	0.34
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD23	9	0.34
(1,2067)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	4	0.34
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	16	0.34
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	15	0.34
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	6	0.34
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	13	0.34
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	6	0.34
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG11	13	0.34
(1,1791)	1:1578:A:ASN:H	1:1592:A:TYR:HH	20	0.34
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	15	0.34
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG3	6	0.34
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	17	0.34
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	20	0.34
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	6	0.34
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	11	0.34
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	3	0.34
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	4	0.34
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	1	0.34
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	3	0.34
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	19	0.34
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	4	0.34
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	13	0.34
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	15	0.34
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	2	0.34
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	17	0.34
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	20	0.34
(1,1330)	1:1569:A:GLN:H	1:1568:A:GLY:HA2	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	3	0.34
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	8	0.34
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG23	5	0.34
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	1	0.34
(1,1174)	1:1591:A:VAL:HG12	1:1592:A:TYR:H	2	0.34
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	19	0.34
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	17	0.34
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	8	0.34
(1,1108)	1:1583:A:TYR:HD1	1:1585:A:ASP:HA	7	0.34
(1,1091)	1:1604:A:LEU:HD21	1:1633:A:THR:HA	10	0.34
(1,1057)	1:1626:A:LEU:HD22	1:1628:A:SER:H	3	0.34
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	5	0.34
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	11	0.34
(1,1056)	1:1626:A:LEU:HD11	1:1636:A:LEU:HB3	10	0.34
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	7	0.34
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	2	0.34
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	3	0.34
(1,1034)	1:1518:A:VAL:HG23	1:1518:A:VAL:HA	8	0.34
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	18	0.34
(1,1019)	1:1625:A:MET:HE1	1:1625:A:MET:HG3	4	0.34
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	19	0.34
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	19	0.34
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	1	0.34
(1,962)	1:1526:A:LEU:HD21	1:1526:A:LEU:HB3	9	0.34
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	20	0.34
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	15	0.34
(1,727)	1:1629:A:LEU:HD22	1:1631:A:LYS:HA	13	0.34
(1,726)	1:1604:A:LEU:HD11	1:1602:A:SER:HA	6	0.34
(1,691)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	9	0.34
(1,674)	1:1581:A:LEU:HD23	1:1529:A:LEU:HD11	8	0.34
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD23	2	0.34
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	8	0.34
(1,599)	1:1587:A:VAL:HG13	1:1611:A:SER:HB2	14	0.34
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE1	15	0.34
(1,569)	1:1547:A:VAL:HG13	1:1539:A:THR:HG22	8	0.34
(1,534)	1:1523:A:THR:HG21	1:1523:A:THR:HA	8	0.34
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	12	0.34
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	5	0.34
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	18	0.34
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	7	0.34
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	1	0.34
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG22	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	1	0.34
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	3	0.34
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	4	0.34
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	10	0.34
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	2	0.34
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD3	4	0.34
(1,266)	2:62:B:THR:HG23	2:63:B:PRO:HG3	6	0.34
(1,245)	2:42:B:ILE:HD13	2:43:B:VAL:HA	1	0.34
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	10	0.34
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	18	0.34
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	19	0.34
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	9	0.34
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	16	0.34
(1,181)	1:1617:A:GLU:H	1:1617:A:GLU:HG3	12	0.34
(1,181)	1:1616:A:PRO:HB3	1:1617:A:GLU:H	16	0.34
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	15	0.34
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	9	0.34
(1,63)	1:1526:A:LEU:HD22	1:1517:A:GLN:HG3	19	0.34
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB3	17	0.34
(1,25)	1:1584:A:VAL:HG11	1:1582:A:ARG:HD2	6	0.34
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	4	0.33
(1,3000)	2:20:B:VAL:H	2:19:B:PHE:HB3	19	0.33
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	1	0.33
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD13	4	0.33
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD23	9	0.33
(1,2785)	2:45:B:GLU:H	2:45:B:GLU:HG3	8	0.33
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	2	0.33
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG22	18	0.33
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	8	0.33
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	7	0.33
(1,2508)	2:14:B:VAL:HG23	2:17:B:LEU:HD12	20	0.33
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	3	0.33
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	18	0.33
(1,2463)	2:56:B:LEU:HD21	2:55:B:LEU:H	12	0.33
(1,2459)	2:56:B:LEU:HD21	2:53:B:LEU:HB2	20	0.33
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	6	0.33
(1,2438)	2:8:B:LEU:HD21	2:8:B:LEU:HA	1	0.33
(1,2437)	2:56:B:LEU:HD11	2:17:B:LEU:HA	11	0.33
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	2	0.33
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG22	1	0.33
(1,2378)	2:42:B:ILE:HG21	2:59:B:TYR:HB3	7	0.33
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE1	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	19	0.33
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	20	0.33
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	6	0.33
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD23	11	0.33
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	7	0.33
(1,2251)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	19	0.33
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	17	0.33
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG22	2	0.33
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	17	0.33
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	18	0.33
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	6	0.33
(1,1837)	1:1618:A:ALA:HB1	1:1622:A:ASN:HD22	14	0.33
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	18	0.33
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	17	0.33
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	9	0.33
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	11	0.33
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	17	0.33
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	20	0.33
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	15	0.33
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	9	0.33
(1,1405)	1:1539:A:THR:HG21	1:1540:A:ALA:H	19	0.33
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	2	0.33
(1,1323)	1:1563:A:VAL:HG21	1:1577:A:ALA:H	1	0.33
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	18	0.33
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	4	0.33
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	17	0.33
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	3	0.33
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD22	5	0.33
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	17	0.33
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	5	0.33
(1,1174)	1:1591:A:VAL:HG13	1:1592:A:TYR:H	6	0.33
(1,1174)	1:1591:A:VAL:HG11	1:1592:A:TYR:H	20	0.33
(1,1157)	1:1581:A:LEU:HD11	1:1581:A:LEU:H	4	0.33
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	15	0.33
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	1	0.33
(1,1089)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	14	0.33
(1,1076)	1:1526:A:LEU:HD11	1:1528:A:ASP:HB3	8	0.33
(1,1072)	1:1590:A:LEU:HD21	1:1553:A:CYS:HA	19	0.33
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	1	0.33
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	18	0.33
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	20	0.33
(1,1044)	1:1518:A:VAL:HG23	1:1582:A:ARG:HA	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:1625:A:MET:HE1	1:1625:A:MET:HG3	16	0.33
(1,1019)	1:1625:A:MET:HE2	1:1625:A:MET:HG3	19	0.33
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	17	0.33
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	11	0.33
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	1	0.33
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD11	10	0.33
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	12	0.33
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	16	0.33
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	9	0.33
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	2	0.33
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	9	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	1	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG21	12	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	14	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	15	0.33
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG21	18	0.33
(1,724)	1:1581:A:LEU:HD23	1:1588:A:LEU:HA	16	0.33
(1,693)	1:1590:A:LEU:HD22	1:1592:A:TYR:HA	11	0.33
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	14	0.33
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	11	0.33
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	14	0.33
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	1	0.33
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	4	0.33
(1,623)	1:1588:A:LEU:HD23	1:1589:A:GLN:H	7	0.33
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	10	0.33
(1,623)	1:1588:A:LEU:HD23	1:1589:A:GLN:H	12	0.33
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	13	0.33
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	9	0.33
(1,603)	1:1519:A:THR:HG23	1:1524:A:GLY:HA3	10	0.33
(1,528)	1:1570:A:THR:HG22	1:1571:A:ARG:H	8	0.33
(1,499)	1:1645:A:ALA:HB3	1:1612:A:PHE:HB2	11	0.33
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	3	0.33
(1,431)	1:1552:A:ILE:HD13	1:1610:A:ILE:HG13	3	0.33
(1,424)	1:1552:A:ILE:HD12	1:1592:A:TYR:HH	10	0.33
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	8	0.33
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	12	0.33
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	17	0.33
(1,387)	1:1572:A:ILE:HD13	2:16:B:THR:H	7	0.33
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD13	7	0.33
(1,367)	1:1593:A:LYS:HE2	1:1580:A:ARG:HE	17	0.33
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	1	0.33
(1,353)	2:61:B:ALA:HB2	2:60:B:CYS:HB2	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	2:55:B:LEU:H	2:55:B:LEU:HD22	15	0.33
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	10	0.33
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	1	0.33
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG22	10	0.33
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	7	0.33
(1,311)	2:46:B:CYS:H	2:42:B:ILE:HG21	10	0.33
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	17	0.33
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	20	0.33
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	5	0.33
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	5	0.33
(1,269)	2:53:B:LEU:HD23	2:53:B:LEU:HA	12	0.33
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	13	0.33
(1,267)	2:35:B:VAL:HG23	2:34:B:ARG:HD3	9	0.33
(1,266)	2:62:B:THR:HG23	2:24:B:ARG:HG3	15	0.33
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	6	0.33
(1,226)	2:17:B:LEU:HD12	2:57:B:GLU:HA	13	0.33
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	18	0.33
(1,218)	1:1567:A:PHE:H	1:1636:A:LEU:HD22	15	0.33
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	1	0.33
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	6	0.33
(1,172)	1:1513:A:HIS:H	1:1514:A:ASP:HB2	2	0.33
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	17	0.33
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	2	0.33
(1,53)	1:1588:A:LEU:HD12	1:1583:A:TYR:H	5	0.33
(1,30)	1:1587:A:VAL:HG22	1:1585:A:ASP:H	3	0.33
(1,30)	1:1587:A:VAL:HG23	1:1585:A:ASP:H	12	0.33
(1,2)	1:1552:A:ILE:HD13	1:1592:A:TYR:HD2	6	0.33
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD23	12	0.32
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	9	0.32
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	16	0.32
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	12	0.32
(1,2841)	2:13:B:LEU:HD22	2:47:B:CYS:H	7	0.32
(1,2832)	2:41:B:GLY:H	2:43:B:VAL:HG13	6	0.32
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG23	10	0.32
(1,2765)	2:43:B:VAL:H	2:42:B:ILE:HG23	2	0.32
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD21	3	0.32
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	7	0.32
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	20	0.32
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	6	0.32
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	16	0.32
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	5	0.32
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	7	0.32
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	16	0.32
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	17	0.32
(1,2500)	2:56:B:LEU:HD22	2:55:B:LEU:HD22	18	0.32
(1,2491)	2:63:B:PRO:HD2	2:62:B:THR:HB	20	0.32
(1,2453)	2:36:B:SER:HB3	2:35:B:VAL:HG13	16	0.32
(1,2448)	2:36:B:SER:HA	2:35:B:VAL:HG12	15	0.32
(1,2439)	2:13:B:LEU:HD22	2:47:B:CYS:H	7	0.32
(1,2438)	2:8:B:LEU:HD22	2:8:B:LEU:HA	9	0.32
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	11	0.32
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	17	0.32
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE1	13	0.32
(1,2305)	2:20:B:VAL:HG11	2:17:B:LEU:HA	9	0.32
(1,2305)	2:20:B:VAL:HG11	2:17:B:LEU:HA	13	0.32
(1,2251)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	5	0.32
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	16	0.32
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG13	12	0.32
(1,2215)	1:1644:A:LEU:HD11	1:1528:A:ASP:H	7	0.32
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	12	0.32
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	16	0.32
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	5	0.32
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	16	0.32
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	1	0.32
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	6	0.32
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	4	0.32
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	5	0.32
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	2	0.32
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	9	0.32
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	17	0.32
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	20	0.32
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	17	0.32
(1,1561)	1:1525:A:HIS:H	1:1520:A:ASN:HB3	14	0.32
(1,1495)	1:1563:A:VAL:HG22	1:1574:A:VAL:H	18	0.32
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	19	0.32
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	5	0.32
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	7	0.32
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	12	0.32
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	2	0.32
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	18	0.32
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	1	0.32
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	6	0.32
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG22	6	0.32
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	5	0.32
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	12	0.32
(1,1331)	1:1569:A:GLN:HG2	1:1569:A:GLN:H	4	0.32
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	5	0.32
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	7	0.32
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	9	0.32
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	11	0.32
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	12	0.32
(1,1283)	1:1601:A:LYS:H	1:1601:A:LYS:HB3	19	0.32
(1,1201)	1:1587:A:VAL:HG23	1:1584:A:VAL:H	12	0.32
(1,1137)	1:1590:A:LEU:HD11	1:1554:A:GLY:H	12	0.32
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	1	0.32
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG11	19	0.32
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD23	13	0.32
(1,1092)	1:1581:A:LEU:HD13	1:1518:A:VAL:H	1	0.32
(1,1091)	1:1604:A:LEU:HD23	1:1633:A:THR:HA	19	0.32
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	12	0.32
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	2	0.32
(1,1045)	1:1587:A:VAL:HG12	1:1587:A:VAL:H	11	0.32
(1,1045)	1:1587:A:VAL:HG11	1:1587:A:VAL:H	12	0.32
(1,1045)	1:1587:A:VAL:HG12	1:1587:A:VAL:H	13	0.32
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	6	0.32
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	6	0.32
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	6	0.32
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	19	0.32
(1,1022)	1:1552:A:ILE:HD12	1:1550:A:MET:HB3	4	0.32
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	3	0.32
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HD1	18	0.32
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	17	0.32
(1,991)	1:1618:A:ALA:HB2	1:1617:A:GLU:HA	14	0.32
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD12	4	0.32
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD21	5	0.32
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	3	0.32
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	17	0.32
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	15	0.32
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG21	7	0.32
(1,774)	1:1509:A:LYS:HB3	1:1508:A:MET:HA	13	0.32
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	3	0.32
(1,748)	1:1513:A:HIS:HB2	1:1512:A:GLU:HA	9	0.32
(1,745)	1:1601:A:LYS:HD3	1:1601:A:LYS:HA	19	0.32
(1,727)	1:1629:A:LEU:HD21	1:1631:A:LYS:HA	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:1581:A:LEU:HD22	1:1588:A:LEU:HA	14	0.32
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	3	0.32
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	4	0.32
(1,659)	1:1526:A:LEU:HD22	1:1527:A:PHE:HA	17	0.32
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	4	0.32
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	19	0.32
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	14	0.32
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	4	0.32
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	7	0.32
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	11	0.32
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	16	0.32
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	19	0.32
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	20	0.32
(1,365)	2:59:B:TYR:H	2:56:B:LEU:HD11	7	0.32
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	5	0.32
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG22	13	0.32
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	16	0.32
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	7	0.32
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	18	0.32
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	18	0.32
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	16	0.32
(1,220)	2:6:B:GLU:HB3	2:2:B:TYR:HE1	3	0.32
(1,220)	2:6:B:GLU:HB3	2:2:B:TYR:HE2	7	0.32
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	7	0.32
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	18	0.32
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB3	3	0.32
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	5	0.32
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	14	0.32
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	12	0.32
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	17	0.32
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD11	13	0.31
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD13	11	0.31
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	20	0.31
(1,2846)	2:17:B:LEU:HD11	2:26:B:PHE:HD2	4	0.31
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB2	4	0.31
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG23	18	0.31
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	10	0.31
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB2	11	0.31
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	6	0.31
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG3	14	0.31
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	5	0.31
(1,2620)	2:37:B:ARG:H	2:32:B:ALA:HB3	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	15	0.31
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG23	11	0.31
(1,2542)	2:50:B:SER:H	2:50:B:SER:HB3	5	0.31
(1,2519)	2:63:B:PRO:HB3	2:62:B:THR:HA	10	0.31
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	1	0.31
(1,2501)	2:56:B:LEU:HD13	2:20:B:VAL:HG11	7	0.31
(1,2480)	2:13:B:LEU:HD12	2:13:B:LEU:HA	9	0.31
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	4	0.31
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	15	0.31
(1,2463)	2:56:B:LEU:HD23	2:55:B:LEU:H	6	0.31
(1,2463)	2:56:B:LEU:HD22	2:55:B:LEU:H	20	0.31
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	3	0.31
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	18	0.31
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	15	0.31
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	16	0.31
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD3	19	0.31
(1,2365)	2:44:B:GLU:HG2	2:43:B:VAL:HG22	14	0.31
(1,2324)	2:64:B:ALA:HB1	2:63:B:PRO:HA	4	0.31
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	16	0.31
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	18	0.31
(1,2286)	2:42:B:ILE:HD13	2:28:B:PHE:HD1	7	0.31
(1,2286)	2:42:B:ILE:HD12	2:28:B:PHE:HD1	18	0.31
(1,2280)	2:42:B:ILE:HD13	2:41:B:GLY:HA3	18	0.31
(1,2278)	2:42:B:ILE:HD11	2:55:B:LEU:HB3	11	0.31
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG21	11	0.31
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG21	18	0.31
(1,2246)	1:1583:A:TYR:HE1	1:1522:A:SER:H	14	0.31
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG12	11	0.31
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	8	0.31
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	8	0.31
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	7	0.31
(1,1992)	1:1523:A:THR:H	1:1521:A:PRO:HG2	10	0.31
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	13	0.31
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	8	0.31
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG11	13	0.31
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG12	17	0.31
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG11	3	0.31
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	19	0.31
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG12	20	0.31
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	12	0.31
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG12	15	0.31
(1,1534)	1:1572:A:ILE:HG22	1:1573:A:SER:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1512)	1:1513:A:HIS:HB3	1:1513:A:HIS:H	17	0.31
(1,1495)	1:1563:A:VAL:HG21	1:1574:A:VAL:H	10	0.31
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	8	0.31
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	4	0.31
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	11	0.31
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	20	0.31
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	10	0.31
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	10	0.31
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	19	0.31
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	2	0.31
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	5	0.31
(1,1200)	1:1584:A:VAL:H	1:1518:A:VAL:HG22	5	0.31
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	11	0.31
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	20	0.31
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG12	5	0.31
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	14	0.31
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	16	0.31
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	10	0.31
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	16	0.31
(1,1019)	1:1625:A:MET:HE2	1:1625:A:MET:HG3	1	0.31
(1,1019)	1:1625:A:MET:HE2	1:1625:A:MET:HG3	11	0.31
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG22	4	0.31
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	20	0.31
(1,1003)	1:1644:A:LEU:HD21	1:1532:A:LEU:H	4	0.31
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	14	0.31
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	7	0.31
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	17	0.31
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	13	0.31
(1,977)	1:1508:A:MET:HE3	1:1508:A:MET:HA	15	0.31
(1,958)	1:1627:A:ILE:HD12	1:1641:A:HIS:HD2	1	0.31
(1,956)	1:1572:A:ILE:HG21	1:1567:A:PHE:HD2	15	0.31
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG11	11	0.31
(1,911)	1:1510:A:SER:HB3	1:1511:A:ASN:H	20	0.31
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	6	0.31
(1,674)	1:1581:A:LEU:HD21	1:1529:A:LEU:HD11	5	0.31
(1,668)	1:1635:A:THR:HG22	1:1607:A:LYS:HG3	17	0.31
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	11	0.31
(1,653)	1:1563:A:VAL:HG21	1:1565:A:ALA:H	1	0.31
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	5	0.31
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	11	0.31
(1,653)	1:1563:A:VAL:HG22	1:1565:A:ALA:H	18	0.31
(1,623)	1:1588:A:LEU:HD21	1:1589:A:GLN:H	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:1626:A:LEU:HD21	1:1636:A:LEU:HB2	17	0.31
(1,599)	1:1587:A:VAL:HG13	1:1611:A:SER:HB2	12	0.31
(1,589)	1:1635:A:THR:HG22	1:1637:A:PHE:HA	9	0.31
(1,583)	1:1540:A:ALA:HB2	1:1638:A:PHE:HE2	11	0.31
(1,564)	1:1591:A:VAL:HG22	1:1593:A:LYS:H	11	0.31
(1,563)	1:1591:A:VAL:HG13	1:1589:A:GLN:HE21	17	0.31
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	9	0.31
(1,512)	1:1645:A:ALA:HB1	1:1614:A:CYS:H	10	0.31
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	19	0.31
(1,458)	1:1572:A:ILE:HD12	1:1572:A:ILE:H	4	0.31
(1,452)	1:1572:A:ILE:HD12	1:1572:A:ILE:HA	20	0.31
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	13	0.31
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	3	0.31
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	6	0.31
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	1	0.31
(1,416)	1:1627:A:ILE:HD11	1:1625:A:MET:HG3	10	0.31
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	12	0.31
(1,411)	1:1602:A:SER:H	1:1600:A:SER:HA	9	0.31
(1,410)	1:1543:A:SER:HB2	1:1547:A:VAL:H	12	0.31
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	10	0.31
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	19	0.31
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG23	7	0.31
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	20	0.31
(1,290)	2:26:B:PHE:H	2:18:B:GLN:H	20	0.31
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	14	0.31
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD22	10	0.31
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	17	0.31
(1,226)	2:17:B:LEU:HD12	2:57:B:GLU:HA	3	0.31
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	11	0.31
(1,203)	1:1598:A:CYS:H	1:1603:A:GLY:HA2	19	0.31
(1,197)	1:1586:A:GLN:H	1:1584:A:VAL:HG22	7	0.31
(1,193)	1:1575:A:GLY:H	1:1606:A:TYR:HB3	14	0.31
(1,183)	1:1608:A:SER:H	1:1591:A:VAL:HG12	8	0.31
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	11	0.31
(1,183)	1:1608:A:SER:H	1:1591:A:VAL:HG11	17	0.31
(1,171)	1:1511:A:ASN:HB2	1:1511:A:ASN:H	6	0.31
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	9	0.31
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	4	0.31
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	14	0.31
(1,67)	1:1601:A:LYS:HG3	1:1600:A:SER:HB2	8	0.31
(1,25)	1:1584:A:VAL:HG11	1:1582:A:ARG:HD3	19	0.31
(1,18)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:1577:A:ALA:HB1	1:1553:A:CYS:H	9	0.31
(1,3019)	2:18:B:GLN:HG3	1:1545:A:SER:HB3	18	0.3
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	16	0.3
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	16	0.3
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE2	16	0.3
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	12	0.3
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD23	8	0.3
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG22	9	0.3
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	13	0.3
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	14	0.3
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	10	0.3
(1,2913)	2:27:B:TYR:HD2	2:27:B:TYR:HA	13	0.3
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	8	0.3
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	10	0.3
(1,2832)	2:41:B:GLY:H	2:43:B:VAL:HG12	3	0.3
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	10	0.3
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG22	14	0.3
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	1	0.3
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	2	0.3
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD21	8	0.3
(1,2686)	2:6:B:GLU:H	2:6:B:GLU:HG2	19	0.3
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	20	0.3
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	5	0.3
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB2	13	0.3
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	6	0.3
(1,2542)	2:50:B:SER:H	2:50:B:SER:HB3	3	0.3
(1,2528)	2:7:B:THR:HG21	2:6:B:GLU:HG3	5	0.3
(1,2522)	2:4:B:PRO:HA	2:2:B:TYR:HD2	2	0.3
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	1	0.3
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	20	0.3
(1,2460)	2:56:B:LEU:HB3	2:56:B:LEU:HD22	7	0.3
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	14	0.3
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	1	0.3
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	7	0.3
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE1	5	0.3
(1,2289)	2:42:B:ILE:HD11	2:55:B:LEU:HD12	19	0.3
(1,2251)	2:55:B:LEU:HD12	2:59:B:TYR:HE2	4	0.3
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG22	16	0.3
(1,2245)	1:1592:A:TYR:HH	1:1590:A:LEU:HD21	2	0.3
(1,2231)	1:1567:A:PHE:HD1	1:1542:A:TYR:HD1	8	0.3
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	16	0.3
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE2	7	0.3
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG13	15	0.3
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	12	0.3
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	11	0.3
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	2	0.3
(1,1585)	1:1550:A:MET:H	1:1548:A:VAL:HG13	20	0.3
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	2	0.3
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	13	0.3
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	14	0.3
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	11	0.3
(1,1496)	1:1574:A:VAL:H	1:1574:A:VAL:HG13	14	0.3
(1,1495)	1:1563:A:VAL:HG21	1:1574:A:VAL:H	1	0.3
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	5	0.3
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	7	0.3
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB3	6	0.3
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	10	0.3
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	4	0.3
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	5	0.3
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	11	0.3
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	5	0.3
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	8	0.3
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	12	0.3
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG12	16	0.3
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	16	0.3
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	14	0.3
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	15	0.3
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	19	0.3
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG21	13	0.3
(1,1203)	1:1588:A:LEU:HD23	1:1584:A:VAL:H	9	0.3
(1,1044)	1:1518:A:VAL:HG22	1:1582:A:ARG:HA	11	0.3
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	9	0.3
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	7	0.3
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	16	0.3
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	10	0.3
(1,987)	1:1627:A:ILE:HD11	1:1638:A:PHE:HA	14	0.3
(1,962)	1:1526:A:LEU:HD23	1:1526:A:LEU:HB3	2	0.3
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	1	0.3
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	1	0.3
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	19	0.3
(1,719)	1:1581:A:LEU:HD13	1:1581:A:LEU:HB3	1	0.3
(1,715)	1:1604:A:LEU:HD21	1:1603:A:GLY:HA2	12	0.3
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD13	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:1635:A:THR:HG23	1:1607:A:LYS:HG3	13	0.3
(1,665)	1:1563:A:VAL:HG21	1:1566:A:CYS:HB3	11	0.3
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	12	0.3
(1,659)	1:1526:A:LEU:HD22	1:1527:A:PHE:HA	13	0.3
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	18	0.3
(1,659)	1:1526:A:LEU:HD21	1:1527:A:PHE:HA	19	0.3
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	10	0.3
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE2	4	0.3
(1,564)	1:1591:A:VAL:HG21	1:1593:A:LYS:H	1	0.3
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	10	0.3
(1,497)	1:1645:A:ALA:HB1	1:1529:A:LEU:HD12	14	0.3
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	14	0.3
(1,440)	1:1550:A:MET:HE3	1:1638:A:PHE:HD2	5	0.3
(1,422)	1:1627:A:ILE:HD11	1:1627:A:ILE:HB	1	0.3
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	10	0.3
(1,420)	1:1627:A:ILE:HD11	1:1639:A:SER:HB2	20	0.3
(1,416)	1:1627:A:ILE:HD12	1:1625:A:MET:HG3	4	0.3
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	4	0.3
(1,365)	2:59:B:TYR:H	2:56:B:LEU:HD12	11	0.3
(1,329)	2:59:B:TYR:HD2	2:42:B:ILE:H	1	0.3
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	13	0.3
(1,266)	2:62:B:THR:HG21	2:63:B:PRO:HG3	4	0.3
(1,263)	2:56:B:LEU:HD21	2:53:B:LEU:HD22	4	0.3
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	11	0.3
(1,246)	2:36:B:SER:HB2	2:33:B:SER:H	10	0.3
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	3	0.3
(1,242)	2:44:B:GLU:HG2	2:48:B:PHE:HB2	20	0.3
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG13	12	0.3
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	13	0.3
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	18	0.3
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	17	0.3
(1,193)	1:1575:A:GLY:H	1:1606:A:TYR:HB3	11	0.3
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	18	0.3
(1,169)	1:1520:A:ASN:H	1:1518:A:VAL:HG12	5	0.3
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	6	0.3
(1,50)	1:1635:A:THR:HG22	1:1609:A:VAL:HB	16	0.3
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	4	0.3
(1,3002)	2:42:B:ILE:HD12	2:28:B:PHE:HE2	13	0.29
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	3	0.29
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	10	0.29
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	18	0.29
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE1	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2848)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	20	0.29
(1,2841)	2:13:B:LEU:HD23	2:47:B:CYS:H	18	0.29
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	16	0.29
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	1	0.29
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	18	0.29
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	12	0.29
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	6	0.29
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	9	0.29
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	18	0.29
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB1	10	0.29
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	9	0.29
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	6	0.29
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	19	0.29
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG3	2	0.29
(1,2552)	2:25:B:GLY:H	2:61:B:ALA:HB1	18	0.29
(1,2540)	2:50:B:SER:H	2:49:B:ARG:HB2	11	0.29
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	6	0.29
(1,2529)	2:43:B:VAL:HG21	2:44:B:GLU:HG3	16	0.29
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	6	0.29
(1,2439)	2:13:B:LEU:HD23	2:47:B:CYS:H	18	0.29
(1,2408)	2:65:B:LYS:HA	2:65:B:LYS:HG2	10	0.29
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD2	7	0.29
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	17	0.29
(1,2324)	2:64:B:ALA:HB3	2:63:B:PRO:HA	7	0.29
(1,2315)	2:43:B:VAL:HG22	2:40:B:ARG:HD3	13	0.29
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	3	0.29
(1,2310)	2:20:B:VAL:HG12	2:21:B:CYS:HB3	17	0.29
(1,2303)	2:20:B:VAL:HG23	2:19:B:PHE:HE2	3	0.29
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	16	0.29
(1,2273)	2:14:B:VAL:HG22	2:26:B:PHE:HB2	13	0.29
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE2	1	0.29
(1,2246)	1:1583:A:TYR:HE1	1:1522:A:SER:H	3	0.29
(1,2185)	1:1558:A:ASN:HD21	1:1549:A:TYR:HD1	15	0.29
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG22	3	0.29
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG21	12	0.29
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG23	19	0.29
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	14	0.29
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	12	0.29
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	15	0.29
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	6	0.29
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	1	0.29
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	11	0.29
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	1	0.29
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	17	0.29
(1,1761)	1:1533:A:SER:H	1:1532:A:LEU:HD13	13	0.29
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	8	0.29
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	20	0.29
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	3	0.29
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	2	0.29
(1,1405)	1:1539:A:THR:HG21	1:1540:A:ALA:H	13	0.29
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	13	0.29
(1,1369)	1:1580:A:ARG:HG2	1:1580:A:ARG:H	7	0.29
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	16	0.29
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	4	0.29
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG23	9	0.29
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	3	0.29
(1,1180)	1:1610:A:ILE:HD11	1:1610:A:ILE:H	8	0.29
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	2	0.29
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	7	0.29
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	19	0.29
(1,1092)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	5	0.29
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	9	0.29
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	19	0.29
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	14	0.29
(1,1024)	1:1552:A:ILE:HD13	1:1590:A:LEU:HD11	2	0.29
(1,1024)	1:1552:A:ILE:HD11	1:1590:A:LEU:HD11	12	0.29
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	7	0.29
(1,974)	1:1533:A:SER:HB3	1:1552:A:ILE:HB	19	0.29
(1,911)	1:1510:A:SER:HB3	1:1511:A:ASN:H	6	0.29
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	13	0.29
(1,751)	1:1635:A:THR:HG23	1:1607:A:LYS:HD3	13	0.29
(1,731)	1:1626:A:LEU:HD13	1:1626:A:LEU:H	5	0.29
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	7	0.29
(1,710)	1:1629:A:LEU:HD11	1:1629:A:LEU:H	6	0.29
(1,705)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	12	0.29
(1,683)	1:1532:A:LEU:HD13	1:1644:A:LEU:HD11	10	0.29
(1,675)	1:1642:A:THR:HG21	1:1613:A:VAL:H	12	0.29
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	2	0.29
(1,596)	1:1529:A:LEU:HD21	1:1645:A:ALA:HA	13	0.29
(1,589)	1:1635:A:THR:HG21	1:1637:A:PHE:HA	7	0.29
(1,579)	1:1519:A:THR:HG21	1:1525:A:HIS:H	13	0.29
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	2	0.29
(1,563)	1:1591:A:VAL:HG13	1:1589:A:GLN:HE21	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:1591:A:VAL:HG12	1:1591:A:VAL:HA	2	0.29
(1,507)	1:1618:A:ALA:HB3	1:1622:A:ASN:HB3	18	0.29
(1,499)	1:1645:A:ALA:HB3	1:1612:A:PHE:HB2	19	0.29
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	5	0.29
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	4	0.29
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	10	0.29
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	1	0.29
(1,446)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	18	0.29
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	17	0.29
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	1	0.29
(1,441)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	18	0.29
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	14	0.29
(1,420)	1:1627:A:ILE:HD13	1:1639:A:SER:HB2	16	0.29
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	13	0.29
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	13	0.29
(1,370)	2:18:B:GLN:HG2	1:1569:A:GLN:HE21	19	0.29
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	15	0.29
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	10	0.29
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	10	0.29
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	5	0.29
(1,315)	2:32:B:ALA:H	2:31:B:PRO:HG3	3	0.29
(1,300)	2:36:B:SER:H	2:32:B:ALA:HB2	6	0.29
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	8	0.29
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	11	0.29
(1,297)	2:37:B:ARG:H	2:33:B:SER:HB2	19	0.29
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	15	0.29
(1,266)	2:62:B:THR:HG23	2:63:B:PRO:HG3	18	0.29
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	8	0.29
(1,228)	2:55:B:LEU:HD21	2:46:B:CYS:HA	5	0.29
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	20	0.29
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	6	0.29
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	16	0.29
(1,169)	1:1512:A:GLU:H	1:1518:A:VAL:HG11	14	0.29
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	13	0.29
(1,114)	1:1542:A:TYR:HE2	1:1629:A:LEU:HB2	5	0.29
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	3	0.29
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	14	0.29
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	4	0.29
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	19	0.29
(1,67)	1:1601:A:LYS:HG3	1:1600:A:SER:HB2	18	0.29
(1,56)	1:1563:A:VAL:HG22	1:1559:A:CYS:H	1	0.29
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG13	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	6	0.29
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	15	0.29
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	5	0.28
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	10	0.28
(1,2974)	2:13:B:LEU:HB2	2:13:B:LEU:HD23	1	0.28
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	20	0.28
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE2	17	0.28
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	14	0.28
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	16	0.28
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	12	0.28
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	19	0.28
(1,2776)	2:55:B:LEU:H	2:55:B:LEU:HD22	11	0.28
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD21	11	0.28
(1,2725)	2:10:B:GLY:H	2:9:B:CYS:HB3	7	0.28
(1,2721)	2:8:B:LEU:H	2:8:B:LEU:HD22	5	0.28
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	7	0.28
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG22	2	0.28
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB3	15	0.28
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	8	0.28
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	13	0.28
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	11	0.28
(1,2525)	2:58:B:THR:HG21	2:59:B:TYR:HE1	14	0.28
(1,2480)	2:13:B:LEU:HD11	2:13:B:LEU:HA	8	0.28
(1,2471)	2:38:B:ARG:H	2:37:B:ARG:HG2	3	0.28
(1,2438)	2:8:B:LEU:HD21	2:8:B:LEU:HA	4	0.28
(1,2352)	2:63:B:PRO:HB2	2:63:B:PRO:HD2	13	0.28
(1,2321)	2:32:B:ALA:HB3	2:33:B:SER:HA	7	0.28
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	19	0.28
(1,2301)	2:20:B:VAL:HG11	2:60:B:CYS:HB2	14	0.28
(1,2295)	2:17:B:LEU:HD23	2:56:B:LEU:HA	4	0.28
(1,2289)	2:42:B:ILE:HD12	2:55:B:LEU:HD11	14	0.28
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	15	0.28
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG21	4	0.28
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG22	5	0.28
(1,2147)	1:1591:A:VAL:HG21	1:1610:A:ILE:H	9	0.28
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	1	0.28
(1,2133)	1:1637:A:PHE:H	1:1636:A:LEU:HD22	13	0.28
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	17	0.28
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	12	0.28
(1,1904)	1:1517:A:GLN:HE21	1:1517:A:GLN:HG2	9	0.28
(1,1904)	1:1517:A:GLN:HE21	1:1517:A:GLN:HG2	15	0.28
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	3	0.28
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	11	0.28
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB3	8	0.28
(1,1789)	1:1577:A:ALA:HB3	1:1578:A:ASN:H	16	0.28
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	11	0.28
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG11	14	0.28
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	19	0.28
(1,1708)	1:1632:A:GLN:HG3	1:1632:A:GLN:H	5	0.28
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	14	0.28
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	6	0.28
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	18	0.28
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD21	2	0.28
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	4	0.28
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	4	0.28
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	1	0.28
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	4	0.28
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	12	0.28
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	8	0.28
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	16	0.28
(1,1373)	1:1572:A:ILE:HG21	1:1572:A:ILE:H	15	0.28
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	16	0.28
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	9	0.28
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	16	0.28
(1,1342)	1:1535:A:ARG:H	1:1534:A:GLY:HA3	18	0.28
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	6	0.28
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	14	0.28
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	8	0.28
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD23	13	0.28
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	4	0.28
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	18	0.28
(1,1064)	1:1529:A:LEU:HD12	1:1588:A:LEU:HB3	20	0.28
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	7	0.28
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	17	0.28
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	11	0.28
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD12	4	0.28
(1,974)	1:1533:A:SER:HB3	1:1552:A:ILE:HB	7	0.28
(1,904)	1:1601:A:LYS:HG3	1:1602:A:SER:HB3	11	0.28
(1,816)	1:1646:A:CYS:HB3	1:1646:A:CYS:HA	16	0.28
(1,745)	1:1601:A:LYS:HD2	1:1601:A:LYS:HA	13	0.28
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD13	9	0.28
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	20	0.28
(1,653)	1:1563:A:VAL:HG21	1:1565:A:ALA:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:1539:A:THR:HG21	1:1558:A:ASN:HD21	13	0.28
(1,623)	1:1588:A:LEU:HD23	1:1589:A:GLN:H	16	0.28
(1,596)	1:1529:A:LEU:HD23	1:1645:A:ALA:HA	12	0.28
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	1	0.28
(1,566)	1:1548:A:VAL:HG23	1:1567:A:PHE:HB3	9	0.28
(1,563)	1:1591:A:VAL:HG11	1:1589:A:GLN:HE21	8	0.28
(1,555)	1:1547:A:VAL:HG13	1:1540:A:ALA:H	4	0.28
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	8	0.28
(1,529)	1:1584:A:VAL:HG13	1:1583:A:TYR:HD1	9	0.28
(1,523)	1:1613:A:VAL:HG22	1:1641:A:HIS:HD2	2	0.28
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	2	0.28
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	15	0.28
(1,458)	1:1572:A:ILE:HD12	1:1572:A:ILE:H	11	0.28
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	17	0.28
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	7	0.28
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	11	0.28
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	15	0.28
(1,400)	2:19:B:PHE:HD1	2:56:B:LEU:HD12	5	0.28
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD11	1	0.28
(1,369)	2:16:B:THR:H	1:1570:A:THR:HG21	11	0.28
(1,363)	1:1632:A:GLN:H	2:53:B:LEU:HD22	14	0.28
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	10	0.28
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	15	0.28
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	9	0.28
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	14	0.28
(1,266)	2:62:B:THR:HG21	2:63:B:PRO:HG3	12	0.28
(1,226)	2:17:B:LEU:HD11	2:57:B:GLU:HA	9	0.28
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	2	0.28
(1,203)	1:1598:A:CYS:H	1:1603:A:GLY:HA2	5	0.28
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	11	0.28
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	10	0.28
(1,183)	1:1608:A:SER:H	1:1591:A:VAL:HG11	18	0.28
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	3	0.28
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	11	0.28
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	19	0.28
(1,144)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	15	0.28
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	7	0.28
(1,55)	1:1518:A:VAL:HG13	1:1511:A:ASN:HB2	1	0.28
(1,28)	1:1609:A:VAL:HG22	1:1607:A:LYS:HB3	1	0.28
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	16	0.27
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	10	0.27
(1,2947)	2:19:B:PHE:HD1	2:20:B:VAL:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	19	0.27
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD1	1	0.27
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD21	7	0.27
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	9	0.27
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	11	0.27
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG22	1	0.27
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	8	0.27
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	18	0.27
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	1	0.27
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG22	10	0.27
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG22	13	0.27
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG23	1	0.27
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD2	14	0.27
(1,2567)	2:18:B:GLN:HE22	2:18:B:GLN:HA	8	0.27
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG11	8	0.27
(1,2541)	2:50:B:SER:H	2:49:B:ARG:HG2	11	0.27
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	2	0.27
(1,2519)	2:63:B:PRO:HB3	2:62:B:THR:HA	13	0.27
(1,2515)	2:55:B:LEU:HD21	2:46:B:CYS:HA	4	0.27
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	6	0.27
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	7	0.27
(1,2507)	2:14:B:VAL:HG23	2:17:B:LEU:HD23	8	0.27
(1,2504)	2:13:B:LEU:HD23	2:9:B:CYS:HB3	3	0.27
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	9	0.27
(1,2463)	2:56:B:LEU:HD22	2:55:B:LEU:H	13	0.27
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	2	0.27
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	12	0.27
(1,2438)	2:8:B:LEU:HD21	2:8:B:LEU:HA	18	0.27
(1,2427)	2:65:B:LYS:H	2:65:B:LYS:HB3	20	0.27
(1,2386)	2:33:B:SER:H	2:33:B:SER:HB3	17	0.27
(1,2373)	2:42:B:ILE:HG22	2:59:B:TYR:HD2	14	0.27
(1,2332)	2:56:B:LEU:HB3	2:17:B:LEU:HG	17	0.27
(1,2324)	2:64:B:ALA:HB3	2:63:B:PRO:HA	16	0.27
(1,2283)	2:42:B:ILE:HD12	2:43:B:VAL:H	17	0.27
(1,2258)	2:43:B:VAL:HG11	2:28:B:PHE:HD2	7	0.27
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG22	15	0.27
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	6	0.27
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	6	0.27
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	10	0.27
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	8	0.27
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	15	0.27
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	2	0.27
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	17	0.27
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	9	0.27
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	11	0.27
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	6	0.27
(1,1909)	1:1589:A:GLN:HE21	1:1587:A:VAL:HG12	8	0.27
(1,1895)	1:1545:A:SER:H	1:1543:A:SER:HB2	15	0.27
(1,1835)	1:1622:A:ASN:HB2	1:1622:A:ASN:HD21	7	0.27
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	7	0.27
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	1	0.27
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	18	0.27
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG23	13	0.27
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	8	0.27
(1,1638)	1:1645:A:ALA:HB1	1:1646:A:CYS:H	10	0.27
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	17	0.27
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	10	0.27
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	9	0.27
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	10	0.27
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	9	0.27
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	14	0.27
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	7	0.27
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	9	0.27
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	16	0.27
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	19	0.27
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG21	8	0.27
(1,1207)	1:1630:A:ASP:H	1:1635:A:THR:HG21	13	0.27
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG22	6	0.27
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	10	0.27
(1,1061)	1:1563:A:VAL:HG13	1:1566:A:CYS:HB3	16	0.27
(1,1057)	1:1626:A:LEU:HD22	1:1628:A:SER:H	13	0.27
(1,1047)	1:1609:A:VAL:HG12	1:1592:A:TYR:H	15	0.27
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	8	0.27
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	9	0.27
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	16	0.27
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	7	0.27
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	10	0.27
(1,802)	1:1607:A:LYS:HB2	1:1607:A:LYS:HE3	7	0.27
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	14	0.27
(1,782)	1:1569:A:GLN:HG2	1:1570:A:THR:H	4	0.27
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG21	9	0.27
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	6	0.27
(1,745)	1:1601:A:LYS:HD3	1:1601:A:LYS:HA	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	2	0.27
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	12	0.27
(1,696)	1:1644:A:LEU:HD21	1:1529:A:LEU:HD23	9	0.27
(1,691)	1:1644:A:LEU:HD21	1:1527:A:PHE:HE1	8	0.27
(1,691)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	16	0.27
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD11	8	0.27
(1,659)	1:1526:A:LEU:HD22	1:1527:A:PHE:HA	15	0.27
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	3	0.27
(1,596)	1:1529:A:LEU:HD23	1:1645:A:ALA:HA	11	0.27
(1,587)	1:1548:A:VAL:HG12	1:1542:A:TYR:HE2	6	0.27
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE2	9	0.27
(1,584)	1:1540:A:ALA:HB3	1:1638:A:PHE:HD1	4	0.27
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	3	0.27
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	2	0.27
(1,531)	1:1591:A:VAL:HG12	1:1591:A:VAL:HA	10	0.27
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	20	0.27
(1,524)	1:1577:A:ALA:HB3	1:1592:A:TYR:HE1	5	0.27
(1,520)	1:1541:A:ALA:HB2	1:1542:A:TYR:HD1	16	0.27
(1,494)	1:1610:A:ILE:HG22	1:1638:A:PHE:HD2	8	0.27
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	19	0.27
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	3	0.27
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	8	0.27
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	10	0.27
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	14	0.27
(1,446)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	16	0.27
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	10	0.27
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	14	0.27
(1,441)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	16	0.27
(1,440)	1:1550:A:MET:HE1	1:1638:A:PHE:HD2	6	0.27
(1,422)	1:1627:A:ILE:HD13	1:1627:A:ILE:HB	2	0.27
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	13	0.27
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	14	0.27
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	20	0.27
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	18	0.27
(1,354)	1:1606:A:TYR:HD2	2:19:B:PHE:HZ	12	0.27
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA3	13	0.27
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	12	0.27
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB2	3	0.27
(1,285)	2:17:B:LEU:HD13	2:27:B:TYR:HD1	12	0.27
(1,269)	2:53:B:LEU:HD22	2:53:B:LEU:HA	4	0.27
(1,260)	2:32:B:ALA:H	2:38:B:ARG:HB3	20	0.27
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB3	20	0.27
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	5	0.27
(1,25)	1:1591:A:VAL:HG12	1:1582:A:ARG:HD3	15	0.27
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	3	0.27
(1,24)	1:1587:A:VAL:HG23	1:1611:A:SER:HB2	20	0.27
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	1	0.27
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	2	0.26
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	3	0.26
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	6	0.26
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	20	0.26
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	14	0.26
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB2	4	0.26
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	17	0.26
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	17	0.26
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	16	0.26
(1,2686)	2:6:B:GLU:H	2:6:B:GLU:HG2	11	0.26
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	13	0.26
(1,2649)	2:40:B:ARG:H	2:40:B:ARG:HG3	17	0.26
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	20	0.26
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD2	9	0.26
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	10	0.26
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	20	0.26
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG3	13	0.26
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	16	0.26
(1,2471)	2:38:B:ARG:H	2:37:B:ARG:HG2	18	0.26
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	1	0.26
(1,2386)	2:33:B:SER:H	2:33:B:SER:HB3	14	0.26
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	17	0.26
(1,2322)	2:32:B:ALA:HB1	2:33:B:SER:HB3	10	0.26
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	10	0.26
(1,2295)	2:17:B:LEU:HD23	2:56:B:LEU:HA	11	0.26
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	1	0.26
(1,2279)	2:42:B:ILE:HD12	2:28:B:PHE:HA	11	0.26
(1,2274)	2:14:B:VAL:HG23	2:18:B:GLN:HG3	13	0.26
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	14	0.26
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG13	16	0.26
(1,2181)	1:1558:A:ASN:HD21	1:1558:A:ASN:H	12	0.26
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	9	0.26
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	5	0.26
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	9	0.26
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	8	0.26
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1973)	1:1600:A:SER:H	1:1599:A:PRO:HG3	13	0.26
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	12	0.26
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	15	0.26
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	9	0.26
(1,1915)	1:1618:A:ALA:HB2	1:1619:A:GLY:H	10	0.26
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD22	12	0.26
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	5	0.26
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	13	0.26
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	16	0.26
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	1	0.26
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	8	0.26
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	19	0.26
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	20	0.26
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	10	0.26
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	16	0.26
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	8	0.26
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG12	5	0.26
(1,1798)	1:1546:A:GLY:H	1:1545:A:SER:HB2	13	0.26
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	18	0.26
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	9	0.26
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	10	0.26
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	4	0.26
(1,1760)	1:1532:A:LEU:HD22	1:1533:A:SER:H	13	0.26
(1,1712)	1:1572:A:ILE:HG21	1:1596:A:SER:H	18	0.26
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	10	0.26
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD23	7	0.26
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	13	0.26
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	3	0.26
(1,1638)	1:1645:A:ALA:HB2	1:1646:A:CYS:H	1	0.26
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	3	0.26
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	19	0.26
(1,1495)	1:1563:A:VAL:HG23	1:1574:A:VAL:H	9	0.26
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	20	0.26
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	17	0.26
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	5	0.26
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	20	0.26
(1,1373)	1:1572:A:ILE:HG23	1:1572:A:ILE:H	12	0.26
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	10	0.26
(1,1355)	1:1621:A:THR:HG21	1:1622:A:ASN:H	17	0.26
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	20	0.26
(1,1328)	1:1552:A:ILE:H	1:1552:A:ILE:HD13	3	0.26
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	13	0.26
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG21	4	0.26
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG21	13	0.26
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	1	0.26
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	2	0.26
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	11	0.26
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	13	0.26
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG23	7	0.26
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG22	12	0.26
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	15	0.26
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	19	0.26
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE1	1	0.26
(1,1070)	1:1588:A:LEU:HD23	1:1583:A:TYR:HE1	16	0.26
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	17	0.26
(1,1028)	1:1610:A:ILE:HG22	1:1612:A:PHE:HD2	7	0.26
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	7	0.26
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	15	0.26
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	3	0.26
(1,980)	1:1625:A:MET:HG3	1:1627:A:ILE:HD13	11	0.26
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	11	0.26
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	19	0.26
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	17	0.26
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	11	0.26
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	12	0.26
(1,724)	1:1581:A:LEU:HD22	1:1588:A:LEU:HA	6	0.26
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD13	13	0.26
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD13	17	0.26
(1,700)	1:1590:A:LEU:HD22	1:1581:A:LEU:HA	1	0.26
(1,696)	1:1644:A:LEU:HD23	1:1529:A:LEU:HD23	15	0.26
(1,680)	1:1529:A:LEU:HD13	1:1588:A:LEU:HD13	7	0.26
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	13	0.26
(1,587)	1:1548:A:VAL:HG13	1:1542:A:TYR:HE2	12	0.26
(1,581)	1:1532:A:LEU:HD21	1:1532:A:LEU:H	3	0.26
(1,566)	1:1548:A:VAL:HG21	1:1567:A:PHE:HB3	19	0.26
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	13	0.26
(1,550)	1:1642:A:THR:HG22	1:1532:A:LEU:HD12	19	0.26
(1,536)	1:1609:A:VAL:HG23	1:1607:A:LYS:HE3	13	0.26
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	9	0.26
(1,490)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	8	0.26
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	10	0.26
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	17	0.26
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:1572:A:ILE:HG21	1:1596:A:SER:HA	9	0.26
(1,470)	1:1572:A:ILE:HG23	1:1596:A:SER:HA	18	0.26
(1,465)	1:1625:A:MET:HE3	1:1625:A:MET:H	11	0.26
(1,458)	1:1572:A:ILE:HD11	1:1572:A:ILE:H	8	0.26
(1,458)	1:1572:A:ILE:HD12	1:1572:A:ILE:H	16	0.26
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	20	0.26
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	13	0.26
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	18	0.26
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	6	0.26
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	15	0.26
(1,442)	1:1550:A:MET:HE2	1:1640:A:TRP:HB2	19	0.26
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	6	0.26
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	15	0.26
(1,424)	1:1552:A:ILE:HD12	1:1592:A:TYR:HH	16	0.26
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	9	0.26
(1,420)	1:1627:A:ILE:HD12	1:1639:A:SER:HB2	3	0.26
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	1	0.26
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	19	0.26
(1,369)	2:16:B:THR:H	1:1570:A:THR:HG21	5	0.26
(1,368)	1:1542:A:TYR:HE1	1:1543:A:SER:HB2	6	0.26
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	9	0.26
(1,363)	1:1632:A:GLN:H	2:53:B:LEU:HD21	10	0.26
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	9	0.26
(1,332)	2:55:B:LEU:HD13	2:56:B:LEU:H	14	0.26
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	9	0.26
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	15	0.26
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	6	0.26
(1,302)	2:40:B:ARG:H	2:41:B:GLY:HA3	3	0.26
(1,297)	2:37:B:ARG:H	2:36:B:SER:HB3	12	0.26
(1,268)	2:56:B:LEU:HD22	2:55:B:LEU:HG	19	0.26
(1,263)	2:56:B:LEU:HD23	2:53:B:LEU:HB3	1	0.26
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	15	0.26
(1,248)	2:36:B:SER:HB3	2:30:B:ARG:HG2	17	0.26
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	10	0.26
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	3	0.26
(1,181)	1:1616:A:PRO:HB3	1:1617:A:GLU:H	6	0.26
(1,171)	1:1511:A:ASN:HB2	1:1511:A:ASN:H	13	0.26
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	13	0.26
(1,87)	1:1584:A:VAL:HG12	1:1585:A:ASP:HB2	11	0.26
(1,36)	1:1540:A:ALA:HB1	1:1548:A:VAL:H	8	0.26
(1,28)	1:1609:A:VAL:HG21	1:1607:A:LYS:HB3	6	0.26
(1,22)	1:1584:A:VAL:HG11	1:1583:A:TYR:H	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:1645:A:ALA:HB1	1:1612:A:PHE:HA	1	0.26
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	13	0.26
(1,11)	1:1625:A:MET:HE1	1:1624:A:PRO:HA	15	0.26
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	7	0.25
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD12	6	0.25
(1,3012)	2:14:B:VAL:H	2:13:B:LEU:HD13	9	0.25
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	3	0.25
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	13	0.25
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	18	0.25
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	9	0.25
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	4	0.25
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	17	0.25
(1,2884)	2:43:B:VAL:HG23	2:28:B:PHE:HD2	19	0.25
(1,2872)	2:17:B:LEU:HD23	2:17:B:LEU:HB2	6	0.25
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD22	11	0.25
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	14	0.25
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB1	19	0.25
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	20	0.25
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	17	0.25
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	12	0.25
(1,2735)	2:56:B:LEU:H	2:54:B:ALA:HB3	5	0.25
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB2	19	0.25
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD2	11	0.25
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD2	15	0.25
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	6	0.25
(1,2591)	2:62:B:THR:H	2:61:B:ALA:HB3	14	0.25
(1,2567)	2:18:B:GLN:HE22	1:1546:A:GLY:HA3	14	0.25
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	13	0.25
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	14	0.25
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG23	2	0.25
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	20	0.25
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	10	0.25
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	10	0.25
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG23	14	0.25
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	18	0.25
(1,2135)	1:1637:A:PHE:H	1:1627:A:ILE:HG12	2	0.25
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	16	0.25
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	20	0.25
(1,1967)	1:1529:A:LEU:H	1:1516:A:CYS:HB2	8	0.25
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	13	0.25
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG12	2	0.25
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	13	0.25
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG22	10	0.25
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	3	0.25
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	8	0.25
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	20	0.25
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	7	0.25
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	17	0.25
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	18	0.25
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	20	0.25
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	20	0.25
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	14	0.25
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	18	0.25
(1,1694)	1:1645:A:ALA:H	1:1644:A:LEU:HB3	11	0.25
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD23	11	0.25
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	20	0.25
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	20	0.25
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	4	0.25
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	9	0.25
(1,1534)	1:1572:A:ILE:HG21	1:1573:A:SER:H	8	0.25
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	20	0.25
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	11	0.25
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	14	0.25
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	16	0.25
(1,1451)	1:1547:A:VAL:HG11	1:1548:A:VAL:H	10	0.25
(1,1405)	1:1539:A:THR:HG21	1:1540:A:ALA:H	18	0.25
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	5	0.25
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	11	0.25
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	9	0.25
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	10	0.25
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG21	20	0.25
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	14	0.25
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	6	0.25
(1,1228)	1:1642:A:THR:HG23	1:1640:A:TRP:HE1	7	0.25
(1,1228)	1:1642:A:THR:HG22	1:1640:A:TRP:HE1	10	0.25
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	18	0.25
(1,1184)	1:1549:A:TYR:H	1:1547:A:VAL:HG22	3	0.25
(1,1157)	1:1581:A:LEU:HD12	1:1581:A:LEU:H	7	0.25
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	7	0.25
(1,1115)	1:1529:A:LEU:HD23	1:1581:A:LEU:HA	19	0.25
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG11	2	0.25
(1,1076)	1:1526:A:LEU:HD12	1:1528:A:ASP:HB3	3	0.25
(1,1034)	1:1518:A:VAL:HG22	1:1518:A:VAL:HA	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	6	0.25
(1,996)	1:1610:A:ILE:HD13	1:1550:A:MET:HG2	11	0.25
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	10	0.25
(1,958)	1:1627:A:ILE:HD11	1:1641:A:HIS:HD2	5	0.25
(1,955)	1:1574:A:VAL:HG12	1:1567:A:PHE:HD1	7	0.25
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	5	0.25
(1,744)	1:1601:A:LYS:HD3	1:1601:A:LYS:H	12	0.25
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	3	0.25
(1,731)	1:1626:A:LEU:HD13	1:1626:A:LEU:H	13	0.25
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	6	0.25
(1,722)	1:1581:A:LEU:HD11	1:1518:A:VAL:HB	3	0.25
(1,722)	1:1581:A:LEU:HD13	1:1518:A:VAL:HB	15	0.25
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	10	0.25
(1,700)	1:1590:A:LEU:HD22	1:1581:A:LEU:HA	6	0.25
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	13	0.25
(1,677)	1:1529:A:LEU:HD13	1:1590:A:LEU:HD13	6	0.25
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	10	0.25
(1,623)	1:1588:A:LEU:HD22	1:1589:A:GLN:H	5	0.25
(1,603)	1:1519:A:THR:HG21	1:1524:A:GLY:HA3	6	0.25
(1,599)	1:1587:A:VAL:HG11	1:1611:A:SER:HB2	11	0.25
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	11	0.25
(1,538)	1:1570:A:THR:HG22	1:1569:A:GLN:HB3	15	0.25
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	5	0.25
(1,531)	1:1591:A:VAL:HG12	1:1591:A:VAL:HA	13	0.25
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	15	0.25
(1,470)	1:1572:A:ILE:HG22	1:1596:A:SER:HA	17	0.25
(1,465)	1:1625:A:MET:HE3	1:1625:A:MET:H	19	0.25
(1,446)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	4	0.25
(1,446)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	5	0.25
(1,444)	1:1550:A:MET:HE2	1:1610:A:ILE:HA	15	0.25
(1,441)	1:1572:A:ILE:HD13	1:1570:A:THR:HB	4	0.25
(1,441)	1:1572:A:ILE:HD11	1:1570:A:THR:HB	5	0.25
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	16	0.25
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD12	12	0.25
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	3	0.25
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	13	0.25
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	17	0.25
(1,344)	2:43:B:VAL:H	2:42:B:ILE:HG12	4	0.25
(1,339)	2:5:B:SER:H	2:5:B:SER:HB2	3	0.25
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	1	0.25
(1,304)	2:9:B:CYS:H	2:13:B:LEU:HD23	16	0.25
(1,288)	2:13:B:LEU:HD22	2:46:B:CYS:HB2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	2:55:B:LEU:HD22	2:46:B:CYS:HA	12	0.25
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	16	0.25
(1,204)	1:1610:A:ILE:HG21	1:1639:A:SER:H	18	0.25
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	2	0.25
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	15	0.25
(1,169)	1:1512:A:GLU:H	1:1518:A:VAL:HG12	19	0.25
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	1	0.25
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	18	0.25
(1,144)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	4	0.25
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	20	0.25
(1,97)	1:1590:A:LEU:HD23	1:1578:A:ASN:H	10	0.25
(1,59)	1:1590:A:LEU:HD21	1:1578:A:ASN:HB2	10	0.25
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	17	0.25
(1,40)	1:1587:A:VAL:HG23	1:1586:A:GLN:HE21	16	0.25
(1,36)	1:1540:A:ALA:HB2	1:1548:A:VAL:H	15	0.25
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	1	0.25
(1,13)	1:1547:A:VAL:HG23	1:1548:A:VAL:HA	4	0.25
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG21	14	0.24
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	16	0.24
(1,2861)	2:20:B:VAL:HG23	2:19:B:PHE:HD2	19	0.24
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	15	0.24
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	7	0.24
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	16	0.24
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	5	0.24
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	2	0.24
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	4	0.24
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	4	0.24
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD3	18	0.24
(1,2554)	2:25:B:GLY:H	2:21:B:CYS:HB3	13	0.24
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD3	19	0.24
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	18	0.24
(1,2521)	2:35:B:VAL:HG23	2:33:B:SER:HB3	8	0.24
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	8	0.24
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	15	0.24
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG23	10	0.24
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	15	0.24
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	17	0.24
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB1	18	0.24
(1,2321)	2:32:B:ALA:HB3	2:33:B:SER:HA	9	0.24
(1,2280)	2:42:B:ILE:HD11	2:41:B:GLY:HA3	16	0.24
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG23	8	0.24
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG23	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	6	0.24
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD13	17	0.24
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD21	10	0.24
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD23	11	0.24
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	1	0.24
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	4	0.24
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	12	0.24
(1,1965)	1:1568:A:GLY:H	1:1549:A:TYR:HE2	4	0.24
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	3	0.24
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	2	0.24
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD22	9	0.24
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	7	0.24
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	15	0.24
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	17	0.24
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	18	0.24
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	3	0.24
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	15	0.24
(1,1847)	1:1602:A:SER:H	1:1601:A:LYS:HG2	19	0.24
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB2	19	0.24
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	5	0.24
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	9	0.24
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	2	0.24
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	6	0.24
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	10	0.24
(1,1574)	1:1518:A:VAL:HG11	1:1519:A:THR:H	18	0.24
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	1	0.24
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	9	0.24
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	7	0.24
(1,1494)	1:1510:A:SER:HB3	1:1511:A:ASN:H	18	0.24
(1,1420)	1:1588:A:LEU:H	1:1612:A:PHE:HB2	12	0.24
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	2	0.24
(1,1364)	1:1600:A:SER:H	1:1600:A:SER:HB2	3	0.24
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	10	0.24
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	1	0.24
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	8	0.24
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	15	0.24
(1,1287)	1:1635:A:THR:HG21	1:1609:A:VAL:H	7	0.24
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	1	0.24
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG22	1	0.24
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	20	0.24
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	16	0.24
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:1529:A:LEU:HD22	1:1581:A:LEU:HA	15	0.24
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG22	6	0.24
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	4	0.24
(1,1064)	1:1529:A:LEU:HD12	1:1588:A:LEU:HB3	7	0.24
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	14	0.24
(1,991)	1:1618:A:ALA:HB3	1:1617:A:GLU:HA	10	0.24
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	18	0.24
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	1	0.24
(1,958)	1:1627:A:ILE:HD12	1:1641:A:HIS:HD2	12	0.24
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	14	0.24
(1,900)	1:1627:A:ILE:HG12	1:1627:A:ILE:HA	15	0.24
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	13	0.24
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	7	0.24
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG23	2	0.24
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG21	4	0.24
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	4	0.24
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	6	0.24
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	3	0.24
(1,722)	1:1581:A:LEU:HD13	1:1518:A:VAL:HB	20	0.24
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	8	0.24
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	16	0.24
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD12	10	0.24
(1,659)	1:1526:A:LEU:HD23	1:1527:A:PHE:HA	7	0.24
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	8	0.24
(1,653)	1:1563:A:VAL:HG23	1:1565:A:ALA:H	9	0.24
(1,652)	1:1581:A:LEU:HD11	1:1527:A:PHE:HD2	5	0.24
(1,635)	1:1539:A:THR:HG23	1:1547:A:VAL:HG22	4	0.24
(1,628)	1:1539:A:THR:HG22	1:1558:A:ASN:HD21	10	0.24
(1,599)	1:1587:A:VAL:HG11	1:1611:A:SER:HB2	13	0.24
(1,579)	1:1519:A:THR:HG21	1:1525:A:HIS:H	7	0.24
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	12	0.24
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	4	0.24
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	20	0.24
(1,542)	1:1613:A:VAL:HG13	1:1641:A:HIS:HA	9	0.24
(1,536)	1:1609:A:VAL:HG23	1:1607:A:LYS:HE3	5	0.24
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	1	0.24
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	6	0.24
(1,531)	1:1591:A:VAL:HG12	1:1591:A:VAL:HA	7	0.24
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	11	0.24
(1,504)	1:1618:A:ALA:HB3	1:1619:A:GLY:HA2	4	0.24
(1,493)	1:1577:A:ALA:HB2	1:1565:A:ALA:H	14	0.24
(1,490)	1:1610:A:ILE:HG21	1:1638:A:PHE:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:1610:A:ILE:HG22	1:1638:A:PHE:H	20	0.24
(1,451)	1:1550:A:MET:HE1	1:1610:A:ILE:HG13	14	0.24
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	17	0.24
(1,446)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	8	0.24
(1,441)	1:1572:A:ILE:HD12	1:1570:A:THR:HB	8	0.24
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	3	0.24
(1,416)	1:1627:A:ILE:HD13	1:1625:A:MET:HG3	11	0.24
(1,402)	1:1629:A:LEU:HB3	2:19:B:PHE:HE2	16	0.24
(1,370)	2:18:B:GLN:HG2	1:1569:A:GLN:HE21	11	0.24
(1,359)	2:58:B:THR:H	2:59:B:TYR:HD2	6	0.24
(1,332)	2:55:B:LEU:HD11	2:56:B:LEU:H	5	0.24
(1,332)	2:55:B:LEU:HD11	2:56:B:LEU:H	6	0.24
(1,310)	2:43:B:VAL:H	2:45:B:GLU:HB2	18	0.24
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	19	0.24
(1,297)	2:37:B:ARG:H	2:33:B:SER:HB2	1	0.24
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	1	0.24
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	5	0.24
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	16	0.24
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	19	0.24
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	2	0.24
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	13	0.24
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	16	0.24
(1,195)	1:1604:A:LEU:HD12	1:1633:A:THR:H	19	0.24
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG21	4	0.24
(1,171)	1:1511:A:ASN:HB2	1:1511:A:ASN:H	11	0.24
(1,169)	1:1512:A:GLU:H	1:1518:A:VAL:HG12	15	0.24
(1,142)	1:1581:A:LEU:HD11	1:1582:A:ARG:HG3	19	0.24
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	12	0.24
(1,67)	1:1601:A:LYS:HG2	1:1600:A:SER:HB2	9	0.24
(1,56)	1:1563:A:VAL:HG21	1:1559:A:CYS:H	11	0.24
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB3	18	0.24
(1,25)	1:1591:A:VAL:HG13	1:1582:A:ARG:HD3	12	0.24
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	15	0.23
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD12	17	0.23
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	19	0.23
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	18	0.23
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG21	3	0.23
(1,2754)	2:12:B:GLU:H	2:8:B:LEU:HD23	20	0.23
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	15	0.23
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD22	20	0.23
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	3	0.23
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	15	0.23
(1,2685)	2:6:B:GLU:H	2:5:B:SER:HA	5	0.23
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB3	2	0.23
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	7	0.23
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	15	0.23
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	20	0.23
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	2	0.23
(1,2459)	2:56:B:LEU:HD22	2:53:B:LEU:HB2	6	0.23
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	7	0.23
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	8	0.23
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	13	0.23
(1,2386)	2:33:B:SER:H	2:33:B:SER:HB3	13	0.23
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	3	0.23
(1,2330)	2:61:B:ALA:HB3	2:60:B:CYS:HA	8	0.23
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	1	0.23
(1,2324)	2:64:B:ALA:HB1	2:63:B:PRO:HA	1	0.23
(1,2251)	2:55:B:LEU:HD13	2:59:B:TYR:HE1	8	0.23
(1,2237)	1:1549:A:TYR:HE1	1:1558:A:ASN:HD22	3	0.23
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG21	17	0.23
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	19	0.23
(1,2147)	1:1591:A:VAL:HG23	1:1610:A:ILE:H	19	0.23
(1,2147)	1:1591:A:VAL:HG21	1:1610:A:ILE:H	20	0.23
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	7	0.23
(1,2105)	1:1612:A:PHE:H	1:1611:A:SER:HB2	6	0.23
(1,2038)	1:1567:A:PHE:H	1:1567:A:PHE:HE2	8	0.23
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	11	0.23
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	9	0.23
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	1	0.23
(1,1928)	1:1575:A:GLY:H	1:1574:A:VAL:HG13	17	0.23
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	8	0.23
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	20	0.23
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	12	0.23
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	19	0.23
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	9	0.23
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	10	0.23
(1,1872)	1:1627:A:ILE:HD11	1:1628:A:SER:H	13	0.23
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	14	0.23
(1,1872)	1:1627:A:ILE:HD13	1:1628:A:SER:H	16	0.23
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	4	0.23
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	9	0.23
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	15	0.23
(1,1802)	1:1546:A:GLY:H	1:1544:A:LYS:HB3	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:1563:A:VAL:HG21	1:1564:A:GLY:H	1	0.23
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	11	0.23
(1,1774)	1:1563:A:VAL:HG22	1:1564:A:GLY:H	18	0.23
(1,1738)	1:1593:A:LYS:HG2	1:1594:A:ASP:H	8	0.23
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	1	0.23
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	12	0.23
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	20	0.23
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	3	0.23
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	10	0.23
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	7	0.23
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	8	0.23
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	7	0.23
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	15	0.23
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	1	0.23
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	4	0.23
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	11	0.23
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	17	0.23
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	16	0.23
(1,1467)	1:1528:A:ASP:H	1:1527:A:PHE:HB3	18	0.23
(1,1457)	1:1514:A:ASP:HB2	1:1514:A:ASP:H	9	0.23
(1,1442)	1:1598:A:CYS:H	1:1597:A:PRO:HG3	6	0.23
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	3	0.23
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	11	0.23
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	15	0.23
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	19	0.23
(1,1333)	1:1569:A:GLN:H	1:1568:A:GLY:H	8	0.23
(1,1301)	1:1557:A:GLU:H	1:1558:A:ASN:HD22	12	0.23
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	5	0.23
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	16	0.23
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	17	0.23
(1,1228)	1:1642:A:THR:HG23	1:1640:A:TRP:HE1	11	0.23
(1,1180)	1:1610:A:ILE:HD11	1:1610:A:ILE:H	9	0.23
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	20	0.23
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	8	0.23
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	19	0.23
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	10	0.23
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	19	0.23
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	20	0.23
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG23	15	0.23
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	4	0.23
(1,987)	1:1627:A:ILE:HD13	1:1638:A:PHE:HA	9	0.23
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD11	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	12	0.23
(1,807)	1:1594:A:ASP:HB3	1:1593:A:LYS:HB2	3	0.23
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	2	0.23
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	16	0.23
(1,726)	1:1604:A:LEU:HD12	1:1602:A:SER:HA	12	0.23
(1,715)	1:1604:A:LEU:HD23	1:1603:A:GLY:HA2	10	0.23
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	4	0.23
(1,626)	1:1539:A:THR:HG22	1:1549:A:TYR:HE1	15	0.23
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	7	0.23
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	10	0.23
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	3	0.23
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	18	0.23
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	9	0.23
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	14	0.23
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	19	0.23
(1,512)	1:1645:A:ALA:HB3	1:1614:A:CYS:H	20	0.23
(1,504)	1:1618:A:ALA:HB2	1:1619:A:GLY:HA2	3	0.23
(1,497)	1:1645:A:ALA:HB1	1:1529:A:LEU:HD12	12	0.23
(1,483)	1:1610:A:ILE:HG23	1:1590:A:LEU:HB3	18	0.23
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	5	0.23
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	12	0.23
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	16	0.23
(1,457)	1:1550:A:MET:HE3	1:1550:A:MET:HA	19	0.23
(1,397)	1:1636:A:LEU:HD11	2:19:B:PHE:HZ	8	0.23
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	5	0.23
(1,396)	1:1542:A:TYR:HD1	2:19:B:PHE:HD1	8	0.23
(1,376)	2:54:B:ALA:HB1	2:52:B:ASP:H	10	0.23
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	18	0.23
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	5	0.23
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	11	0.23
(1,332)	2:55:B:LEU:HD11	2:56:B:LEU:H	19	0.23
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	4	0.23
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG3	16	0.23
(1,272)	2:54:B:ALA:HB1	2:55:B:LEU:HB2	11	0.23
(1,266)	2:62:B:THR:HG21	2:63:B:PRO:HG3	7	0.23
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	16	0.23
(1,232)	2:55:B:LEU:HD22	2:46:B:CYS:HB3	2	0.23
(1,228)	2:55:B:LEU:HD23	2:46:B:CYS:HA	20	0.23
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	17	0.23
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	10	0.23
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	17	0.23
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	17	0.23
(1,149)	1:1638:A:PHE:HD1	1:1540:A:ALA:HB1	12	0.23
(1,139)	1:1610:A:ILE:HD12	1:1590:A:LEU:HD21	12	0.23
(1,116)	1:1613:A:VAL:HG11	1:1642:A:THR:H	6	0.23
(1,103)	1:1610:A:ILE:HD11	1:1590:A:LEU:H	13	0.23
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	15	0.23
(1,97)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	11	0.23
(1,46)	1:1540:A:ALA:HB2	1:1541:A:ALA:HA	9	0.23
(1,32)	1:1547:A:VAL:HG22	1:1567:A:PHE:HB3	6	0.23
(1,32)	1:1547:A:VAL:HG23	1:1549:A:TYR:HB3	10	0.23
(1,18)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	17	0.23
(1,18)	1:1645:A:ALA:HB3	1:1646:A:CYS:HB2	20	0.23
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	5	0.23
(1,15)	1:1577:A:ALA:HB1	1:1555:A:GLU:HG2	17	0.23
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG12	7	0.22
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD21	10	0.22
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD13	5	0.22
(1,2938)	2:17:B:LEU:H	2:56:B:LEU:HD11	8	0.22
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	14	0.22
(1,2861)	2:20:B:VAL:HG21	2:19:B:PHE:HD2	1	0.22
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	15	0.22
(1,2846)	2:17:B:LEU:HD13	2:26:B:PHE:HD2	2	0.22
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB3	18	0.22
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG22	20	0.22
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	2	0.22
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	8	0.22
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	16	0.22
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD23	7	0.22
(1,2726)	2:10:B:GLY:H	2:13:B:LEU:HD21	18	0.22
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	16	0.22
(1,2699)	2:3:B:ARG:H	2:3:B:ARG:HB3	14	0.22
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB2	17	0.22
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB3	9	0.22
(1,2645)	2:41:B:GLY:H	2:40:B:ARG:HD3	10	0.22
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	18	0.22
(1,2543)	2:50:B:SER:H	2:49:B:ARG:HD2	16	0.22
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG22	5	0.22
(1,2528)	2:7:B:THR:HG23	2:6:B:GLU:HG3	14	0.22
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	12	0.22
(1,2463)	2:56:B:LEU:HD22	2:55:B:LEU:H	19	0.22
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	7	0.22
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	18	0.22
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	1	0.22
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	15	0.22
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	2	0.22
(1,2373)	2:42:B:ILE:HG23	2:59:B:TYR:HD1	15	0.22
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	18	0.22
(1,2315)	2:43:B:VAL:HG23	2:40:B:ARG:HD2	2	0.22
(1,2274)	2:14:B:VAL:HG22	2:18:B:GLN:HG3	12	0.22
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG21	11	0.22
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG11	20	0.22
(1,2215)	1:1644:A:LEU:HD12	1:1528:A:ASP:H	3	0.22
(1,2139)	1:1640:A:TRP:H	1:1613:A:VAL:HG13	18	0.22
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	3	0.22
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	19	0.22
(1,1925)	1:1575:A:GLY:H	1:1595:A:GLY:HA2	15	0.22
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG23	2	0.22
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG11	5	0.22
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD23	15	0.22
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	4	0.22
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	5	0.22
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG21	13	0.22
(1,1804)	1:1511:A:ASN:HD22	1:1518:A:VAL:HG12	14	0.22
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD13	17	0.22
(1,1782)	1:1517:A:GLN:H	1:1515:A:ASP:HB2	4	0.22
(1,1774)	1:1563:A:VAL:HG23	1:1564:A:GLY:H	8	0.22
(1,1710)	1:1632:A:GLN:H	1:1631:A:LYS:HB2	18	0.22
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	1	0.22
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	12	0.22
(1,1574)	1:1518:A:VAL:HG12	1:1519:A:THR:H	16	0.22
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG3	19	0.22
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	9	0.22
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	13	0.22
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	16	0.22
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	6	0.22
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	7	0.22
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	2	0.22
(1,1454)	1:1610:A:ILE:HG21	1:1611:A:SER:H	9	0.22
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	18	0.22
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG23	17	0.22
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	19	0.22
(1,1301)	1:1557:A:GLU:H	1:1558:A:ASN:HD22	2	0.22
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:1635:A:THR:HG22	1:1609:A:VAL:H	9	0.22
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	6	0.22
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	18	0.22
(1,1203)	1:1588:A:LEU:HD23	1:1584:A:VAL:H	12	0.22
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG3	2	0.22
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	4	0.22
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	10	0.22
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	11	0.22
(1,1042)	1:1609:A:VAL:HG12	1:1637:A:PHE:HB3	18	0.22
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	8	0.22
(1,1003)	1:1644:A:LEU:HD21	1:1532:A:LEU:H	19	0.22
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	11	0.22
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	15	0.22
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	2	0.22
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	9	0.22
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	11	0.22
(1,968)	1:1521:A:PRO:HG2	1:1522:A:SER:H	3	0.22
(1,823)	1:1623:A:ARG:HD2	1:1623:A:ARG:HE	18	0.22
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	18	0.22
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG23	13	0.22
(1,770)	1:1521:A:PRO:HB2	1:1522:A:SER:HB2	3	0.22
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	1	0.22
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	11	0.22
(1,736)	1:1626:A:LEU:HD11	1:1626:A:LEU:HB3	18	0.22
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD13	17	0.22
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD11	2	0.22
(1,674)	1:1581:A:LEU:HD22	1:1529:A:LEU:HD12	18	0.22
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	18	0.22
(1,663)	1:1563:A:VAL:HG21	1:1559:A:CYS:HB2	20	0.22
(1,637)	1:1518:A:VAL:HG12	1:1581:A:LEU:HD23	13	0.22
(1,583)	1:1540:A:ALA:HB1	1:1638:A:PHE:HE1	10	0.22
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	6	0.22
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	16	0.22
(1,542)	1:1613:A:VAL:HG11	1:1641:A:HIS:HA	6	0.22
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	4	0.22
(1,531)	1:1591:A:VAL:HG11	1:1591:A:VAL:HA	12	0.22
(1,490)	1:1610:A:ILE:HG23	1:1638:A:PHE:H	9	0.22
(1,485)	1:1577:A:ALA:HB3	1:1564:A:GLY:HA3	7	0.22
(1,458)	1:1572:A:ILE:HD11	1:1572:A:ILE:H	10	0.22
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	20	0.22
(1,445)	1:1550:A:MET:HE1	1:1638:A:PHE:HB3	6	0.22
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	2:19:B:PHE:HD2	2:16:B:THR:HG23	12	0.22
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD13	19	0.22
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	1	0.22
(1,366)	2:28:B:PHE:HE2	2:28:B:PHE:HA	2	0.22
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	18	0.22
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	15	0.22
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	9	0.22
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	8	0.22
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	2	0.22
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	20	0.22
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	12	0.22
(1,248)	2:29:B:SER:HB2	2:30:B:ARG:HG2	18	0.22
(1,245)	2:42:B:ILE:HD11	2:14:B:VAL:HA	20	0.22
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG11	7	0.22
(1,232)	2:55:B:LEU:HD21	2:46:B:CYS:HB3	3	0.22
(1,230)	2:55:B:LEU:HD12	2:59:B:TYR:H	10	0.22
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB2	11	0.22
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	12	0.22
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	7	0.22
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	16	0.22
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	1	0.22
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	2	0.22
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	9	0.22
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	8	0.22
(1,149)	1:1638:A:PHE:HD1	1:1540:A:ALA:HB1	5	0.22
(1,142)	1:1581:A:LEU:HD13	1:1582:A:ARG:HG3	10	0.22
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	7	0.22
(1,49)	1:1540:A:ALA:HB3	1:1625:A:MET:HG2	6	0.22
(1,40)	1:1587:A:VAL:HG22	1:1586:A:GLN:HE21	15	0.22
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	3	0.22
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD23	3	0.21
(1,3008)	2:56:B:LEU:HD21	2:17:B:LEU:H	15	0.21
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	20	0.21
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	1	0.21
(1,2913)	2:27:B:TYR:HD2	2:27:B:TYR:HA	1	0.21
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD23	10	0.21
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD23	4	0.21
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	13	0.21
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG21	19	0.21
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	1	0.21
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD22	20	0.21
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD3	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2660)	2:64:B:ALA:H	2:63:B:PRO:HG2	18	0.21
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG23	11	0.21
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB1	8	0.21
(1,2652)	2:40:B:ARG:H	2:39:B:SER:HB3	2	0.21
(1,2642)	2:41:B:GLY:H	2:40:B:ARG:HG2	6	0.21
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	12	0.21
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	20	0.21
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	12	0.21
(1,2607)	2:34:B:ARG:H	2:34:B:ARG:HG2	14	0.21
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	20	0.21
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	7	0.21
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG23	4	0.21
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG21	3	0.21
(1,2524)	2:64:B:ALA:HA	2:65:B:LYS:HB2	1	0.21
(1,2524)	2:64:B:ALA:HA	2:65:B:LYS:HB2	10	0.21
(1,2523)	2:64:B:ALA:HA	2:63:B:PRO:HB3	14	0.21
(1,2521)	2:35:B:VAL:HG22	2:33:B:SER:HB3	4	0.21
(1,2521)	2:35:B:VAL:HG23	2:33:B:SER:HB3	9	0.21
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	13	0.21
(1,2438)	2:8:B:LEU:HD22	2:8:B:LEU:HA	17	0.21
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	9	0.21
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG11	11	0.21
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	12	0.21
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	1	0.21
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	12	0.21
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB3	8	0.21
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE1	4	0.21
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB1	14	0.21
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB2	14	0.21
(1,2234)	1:1592:A:TYR:HE1	1:1577:A:ALA:HB3	14	0.21
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG12	9	0.21
(1,2215)	1:1644:A:LEU:HD12	1:1528:A:ASP:H	16	0.21
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG21	18	0.21
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	20	0.21
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	10	0.21
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG11	8	0.21
(1,2067)	1:1590:A:LEU:HD23	1:1578:A:ASN:H	10	0.21
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	13	0.21
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	10	0.21
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	14	0.21
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	7	0.21
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	6	0.21
(1,1927)	1:1563:A:VAL:HG21	1:1575:A:GLY:H	1	0.21
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	4	0.21
(1,1927)	1:1563:A:VAL:HG21	1:1575:A:GLY:H	10	0.21
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	1	0.21
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	3	0.21
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	10	0.21
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	16	0.21
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	1	0.21
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	10	0.21
(1,1872)	1:1627:A:ILE:HD12	1:1628:A:SER:H	2	0.21
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	9	0.21
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	17	0.21
(1,1785)	1:1517:A:GLN:H	1:1517:A:GLN:HG2	12	0.21
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG12	15	0.21
(1,1774)	1:1563:A:VAL:HG21	1:1564:A:GLY:H	10	0.21
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	11	0.21
(1,1638)	1:1645:A:ALA:HB2	1:1646:A:CYS:H	15	0.21
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	3	0.21
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	4	0.21
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	5	0.21
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	15	0.21
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	1	0.21
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	6	0.21
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	15	0.21
(1,1471)	1:1551:A:SER:H	1:1550:A:MET:HG2	6	0.21
(1,1468)	1:1528:A:ASP:HB2	1:1528:A:ASP:H	15	0.21
(1,1457)	1:1514:A:ASP:HB2	1:1514:A:ASP:H	7	0.21
(1,1420)	1:1588:A:LEU:H	1:1612:A:PHE:HB2	11	0.21
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	10	0.21
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	2	0.21
(1,1228)	1:1642:A:THR:HG21	1:1640:A:TRP:HE1	17	0.21
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG21	16	0.21
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	11	0.21
(1,1047)	1:1609:A:VAL:HG13	1:1592:A:TYR:H	4	0.21
(1,1011)	1:1542:A:TYR:HD1	1:1543:A:SER:HB3	4	0.21
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	13	0.21
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	19	0.21
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	6	0.21
(1,958)	1:1627:A:ILE:HD11	1:1641:A:HIS:HD2	20	0.21
(1,935)	1:1636:A:LEU:HD11	1:1636:A:LEU:H	4	0.21
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	20	0.21
(1,777)	1:1649:A:GLU:HG2	1:1649:A:GLU:HA	20	0.21
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	20	0.21
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	19	0.21
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	2	0.21
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	4	0.21
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	8	0.21
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	14	0.21
(1,707)	1:1590:A:LEU:HD13	1:1592:A:TYR:HE1	16	0.21
(1,696)	1:1644:A:LEU:HD21	1:1529:A:LEU:HD23	10	0.21
(1,589)	1:1635:A:THR:HG22	1:1637:A:PHE:HA	3	0.21
(1,586)	1:1548:A:VAL:HG22	1:1638:A:PHE:HD1	15	0.21
(1,581)	1:1532:A:LEU:HD23	1:1532:A:LEU:H	2	0.21
(1,566)	1:1548:A:VAL:HG22	1:1567:A:PHE:HB3	14	0.21
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	1	0.21
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	14	0.21
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	16	0.21
(1,528)	1:1570:A:THR:HG23	1:1571:A:ARG:H	12	0.21
(1,458)	1:1572:A:ILE:HD11	1:1572:A:ILE:H	6	0.21
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	1	0.21
(1,442)	1:1550:A:MET:HE1	1:1640:A:TRP:HB2	3	0.21
(1,420)	1:1627:A:ILE:HD13	1:1639:A:SER:HB2	8	0.21
(1,420)	1:1627:A:ILE:HD13	1:1639:A:SER:HB2	11	0.21
(1,386)	1:1572:A:ILE:HD11	2:12:B:GLU:HA	12	0.21
(1,379)	1:1632:A:GLN:HG2	2:53:B:LEU:HD23	15	0.21
(1,353)	2:61:B:ALA:HB2	2:60:B:CYS:HB2	12	0.21
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	7	0.21
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG23	14	0.21
(1,239)	2:17:B:LEU:H	2:20:B:VAL:HG12	11	0.21
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	19	0.21
(1,204)	1:1610:A:ILE:HG23	1:1639:A:SER:H	17	0.21
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG22	1	0.21
(1,168)	1:1512:A:GLU:HB3	1:1512:A:GLU:H	20	0.21
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	5	0.21
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	7	0.21
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	20	0.21
(1,142)	1:1581:A:LEU:HD12	1:1582:A:ARG:HG3	20	0.21
(1,116)	1:1613:A:VAL:HG13	1:1642:A:THR:H	2	0.21
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	18	0.21
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	1	0.21
(1,47)	1:1518:A:VAL:HG12	1:1513:A:HIS:HB2	16	0.21
(1,24)	1:1587:A:VAL:HG21	1:1586:A:GLN:HA	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:1645:A:ALA:HB3	1:1612:A:PHE:HA	19	0.21
(1,9)	1:1550:A:MET:HE2	1:1551:A:SER:H	18	0.21
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	8	0.21
(2,2)	1:1575:A:GLY:H	1:1563:A:VAL:HG13	14	0.2
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	12	0.2
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD23	10	0.2
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD13	14	0.2
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD23	16	0.2
(1,2961)	2:56:B:LEU:HD23	2:53:B:LEU:H	3	0.2
(1,2923)	2:28:B:PHE:H	2:27:B:TYR:HD1	13	0.2
(1,2860)	2:17:B:LEU:HD13	2:28:B:PHE:HE2	12	0.2
(1,2831)	2:41:B:GLY:H	2:42:B:ILE:HG12	6	0.2
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG13	18	0.2
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	19	0.2
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD11	4	0.2
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	9	0.2
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	16	0.2
(1,2621)	2:37:B:ARG:H	2:37:B:ARG:HD3	20	0.2
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	11	0.2
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	15	0.2
(1,2538)	2:13:B:LEU:HD11	2:43:B:VAL:HA	16	0.2
(1,2531)	2:61:B:ALA:HB1	2:62:B:THR:HA	12	0.2
(1,2528)	2:7:B:THR:HG22	2:6:B:GLU:HG3	8	0.2
(1,2525)	2:58:B:THR:HG22	2:59:B:TYR:HE1	10	0.2
(1,2471)	2:38:B:ARG:H	2:37:B:ARG:HG2	6	0.2
(1,2458)	2:7:B:THR:HG21	2:6:B:GLU:HB2	17	0.2
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	4	0.2
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	7	0.2
(1,2373)	2:42:B:ILE:HG23	2:59:B:TYR:HD1	17	0.2
(1,2372)	2:30:B:ARG:HD2	2:59:B:TYR:HE2	12	0.2
(1,2324)	2:64:B:ALA:HB2	2:63:B:PRO:HA	5	0.2
(1,2310)	2:20:B:VAL:HG13	2:21:B:CYS:HB3	7	0.2
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	9	0.2
(1,2286)	2:42:B:ILE:HD12	2:28:B:PHE:HD2	17	0.2
(1,2260)	2:28:B:PHE:HD2	2:42:B:ILE:HG13	7	0.2
(1,2249)	2:28:B:PHE:HD1	2:43:B:VAL:HG22	3	0.2
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	3	0.2
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG22	18	0.2
(1,2169)	1:1589:A:GLN:HE22	1:1589:A:GLN:HB3	16	0.2
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	15	0.2
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD12	16	0.2
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	6	0.2
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	18	0.2
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	7	0.2
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	17	0.2
(1,1927)	1:1563:A:VAL:HG22	1:1575:A:GLY:H	18	0.2
(1,1915)	1:1618:A:ALA:HB1	1:1619:A:GLY:H	15	0.2
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG12	18	0.2
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	11	0.2
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG21	1	0.2
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	18	0.2
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD22	17	0.2
(1,1749)	1:1605:A:SER:H	1:1605:A:SER:HB2	8	0.2
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	14	0.2
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	16	0.2
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	15	0.2
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	16	0.2
(1,1638)	1:1645:A:ALA:HB2	1:1646:A:CYS:H	5	0.2
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	12	0.2
(1,1636)	1:1559:A:CYS:H	1:1558:A:ASN:HB2	12	0.2
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG21	6	0.2
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	5	0.2
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	8	0.2
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	14	0.2
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	6	0.2
(1,1489)	1:1551:A:SER:H	1:1551:A:SER:HB3	19	0.2
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD13	3	0.2
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD12	16	0.2
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	18	0.2
(1,1455)	1:1513:A:HIS:HB3	1:1514:A:ASP:H	12	0.2
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG23	2	0.2
(1,1369)	1:1580:A:ARG:HG3	1:1580:A:ARG:H	3	0.2
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG22	4	0.2
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG23	4	0.2
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	16	0.2
(1,1237)	1:1540:A:ALA:HB2	1:1541:A:ALA:H	9	0.2
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	5	0.2
(1,1139)	1:1577:A:ALA:HB2	1:1554:A:GLY:H	6	0.2
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	15	0.2
(1,1120)	1:1526:A:LEU:HB3	1:1526:A:LEU:H	7	0.2
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	2	0.2
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	1	0.2
(1,1045)	1:1587:A:VAL:HG13	1:1587:A:VAL:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:1609:A:VAL:HG11	1:1637:A:PHE:HB3	4	0.2
(1,1029)	1:1610:A:ILE:HG23	1:1640:A:TRP:HZ3	18	0.2
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	2	0.2
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	5	0.2
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	5	0.2
(1,932)	1:1601:A:LYS:HD3	1:1604:A:LEU:HD13	12	0.2
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	11	0.2
(1,884)	1:1649:A:GLU:HB2	1:1649:A:GLU:HA	18	0.2
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	8	0.2
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG22	3	0.2
(1,787)	1:1617:A:GLU:HG2	1:1617:A:GLU:HA	10	0.2
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	16	0.2
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	11	0.2
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	13	0.2
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	17	0.2
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	10	0.2
(1,731)	1:1626:A:LEU:HD13	1:1626:A:LEU:H	17	0.2
(1,722)	1:1581:A:LEU:HD12	1:1518:A:VAL:HB	9	0.2
(1,722)	1:1581:A:LEU:HD11	1:1518:A:VAL:HB	10	0.2
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	1	0.2
(1,700)	1:1590:A:LEU:HD23	1:1581:A:LEU:HA	16	0.2
(1,696)	1:1644:A:LEU:HD22	1:1529:A:LEU:HD23	1	0.2
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	6	0.2
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	16	0.2
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	5	0.2
(1,553)	1:1541:A:ALA:HB3	1:1540:A:ALA:HA	6	0.2
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	7	0.2
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	12	0.2
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	17	0.2
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	5	0.2
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	6	0.2
(1,467)	1:1625:A:MET:HE3	1:1625:A:MET:HA	15	0.2
(1,465)	1:1625:A:MET:HE2	1:1625:A:MET:H	16	0.2
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	18	0.2
(1,457)	1:1550:A:MET:HE2	1:1550:A:MET:HA	3	0.2
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	17	0.2
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	12	0.2
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	13	0.2
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	2	0.2
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	3	0.2
(1,317)	2:53:B:LEU:H	2:55:B:LEU:HB3	11	0.2
(1,298)	2:36:B:SER:H	2:34:B:ARG:HB3	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	2:54:B:ALA:H	2:53:B:LEU:HD22	11	0.2
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	14	0.2
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	10	0.2
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	14	0.2
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	11	0.2
(1,147)	1:1638:A:PHE:HD2	1:1610:A:ILE:HD11	18	0.2
(1,114)	1:1542:A:TYR:HE1	1:1629:A:LEU:HB2	15	0.2
(1,111)	1:1595:A:GLY:HA3	1:1596:A:SER:HB2	16	0.2
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	3	0.2
(1,46)	1:1540:A:ALA:HB3	1:1541:A:ALA:HA	10	0.2
(1,32)	1:1547:A:VAL:HG22	1:1549:A:TYR:HB3	9	0.2
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG13	7	0.2
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	10	0.2
(3,18)	1:1547:A:VAL:O	1:1568:A:GLY:N	8	0.19
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	17	0.19
(1,3011)	2:13:B:LEU:HB3	2:13:B:LEU:H	6	0.19
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	15	0.19
(1,2860)	2:17:B:LEU:HD13	2:28:B:PHE:HE2	10	0.19
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	17	0.19
(1,2836)	2:9:B:CYS:H	2:13:B:LEU:HB2	19	0.19
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	5	0.19
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB3	17	0.19
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB3	18	0.19
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG21	3	0.19
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	10	0.19
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	15	0.19
(1,2798)	2:62:B:THR:H	2:24:B:ARG:HG3	18	0.19
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD21	17	0.19
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	1	0.19
(1,2775)	2:65:B:LYS:H	2:62:B:THR:HG23	16	0.19
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD1	14	0.19
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	3	0.19
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	8	0.19
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	14	0.19
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	9	0.19
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	20	0.19
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	3	0.19
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB2	19	0.19
(1,2629)	2:36:B:SER:H	2:35:B:VAL:HB	10	0.19
(1,2616)	2:35:B:VAL:H	2:33:B:SER:HB2	10	0.19
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	10	0.19
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD3	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	6	0.19
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	13	0.19
(1,2552)	2:25:B:GLY:H	2:61:B:ALA:HB1	17	0.19
(1,2537)	2:13:B:LEU:HD21	2:9:B:CYS:HB3	8	0.19
(1,2519)	2:63:B:PRO:HB3	2:62:B:THR:HA	20	0.19
(1,2515)	2:55:B:LEU:HD21	2:46:B:CYS:HA	5	0.19
(1,2506)	2:56:B:LEU:HD11	2:20:B:VAL:H	16	0.19
(1,2504)	2:13:B:LEU:HD22	2:9:B:CYS:HB3	10	0.19
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	18	0.19
(1,2481)	2:13:B:LEU:HD12	2:14:B:VAL:HB	8	0.19
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	8	0.19
(1,2459)	2:56:B:LEU:HD21	2:53:B:LEU:HB2	13	0.19
(1,2454)	2:35:B:VAL:HG22	2:34:B:ARG:HA	13	0.19
(1,2430)	2:63:B:PRO:HD2	2:63:B:PRO:HB3	20	0.19
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	15	0.19
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	14	0.19
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB1	15	0.19
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG23	19	0.19
(1,2295)	2:17:B:LEU:HD21	2:56:B:LEU:HA	17	0.19
(1,2291)	2:17:B:LEU:HD12	2:17:B:LEU:HA	6	0.19
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG23	4	0.19
(1,2246)	1:1583:A:TYR:HE2	1:1522:A:SER:H	20	0.19
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG23	6	0.19
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	10	0.19
(1,2067)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	11	0.19
(1,2053)	1:1573:A:SER:H	1:1563:A:VAL:HG21	7	0.19
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	7	0.19
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	5	0.19
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	16	0.19
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	1	0.19
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD23	17	0.19
(1,1880)	1:1533:A:SER:HB2	1:1534:A:GLY:H	14	0.19
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	2	0.19
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	17	0.19
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG13	13	0.19
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	12	0.19
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	15	0.19
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	17	0.19
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	8	0.19
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD21	12	0.19
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	2	0.19
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	2	0.19
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB2	3	0.19
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	4	0.19
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	14	0.19
(1,1421)	1:1588:A:LEU:H	1:1645:A:ALA:HB2	20	0.19
(1,1395)	1:1591:A:VAL:H	1:1590:A:LEU:HB3	1	0.19
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	16	0.19
(1,1345)	1:1535:A:ARG:HD2	1:1535:A:ARG:H	16	0.19
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	11	0.19
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	16	0.19
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG21	8	0.19
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	7	0.19
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	15	0.19
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	19	0.19
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG2	6	0.19
(1,1139)	1:1577:A:ALA:HB1	1:1554:A:GLY:H	9	0.19
(1,1137)	1:1590:A:LEU:HD11	1:1554:A:GLY:H	17	0.19
(1,1120)	1:1526:A:LEU:HB3	1:1526:A:LEU:H	13	0.19
(1,1094)	1:1588:A:LEU:HD13	1:1581:A:LEU:HG	11	0.19
(1,1072)	1:1590:A:LEU:HD22	1:1553:A:CYS:HA	4	0.19
(1,1042)	1:1609:A:VAL:HG12	1:1637:A:PHE:HB3	20	0.19
(1,1034)	1:1518:A:VAL:HG21	1:1518:A:VAL:HA	15	0.19
(1,1031)	1:1577:A:ALA:HB2	1:1562:A:GLY:HA3	9	0.19
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	13	0.19
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	8	0.19
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	9	0.19
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	16	0.19
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	18	0.19
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	4	0.19
(1,787)	1:1617:A:GLU:HG2	1:1617:A:GLU:HA	7	0.19
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	5	0.19
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	6	0.19
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	15	0.19
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	4	0.19
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	14	0.19
(1,706)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	18	0.19
(1,705)	1:1581:A:LEU:HD13	1:1518:A:VAL:H	20	0.19
(1,700)	1:1590:A:LEU:HD21	1:1581:A:LEU:HA	10	0.19
(1,697)	1:1644:A:LEU:HD11	1:1529:A:LEU:HD12	17	0.19
(1,680)	1:1529:A:LEU:HD11	1:1588:A:LEU:HD12	9	0.19
(1,643)	1:1604:A:LEU:HD11	1:1633:A:THR:H	12	0.19
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	10	0.19
(1,603)	1:1519:A:THR:HG22	1:1524:A:GLY:HA3	1	0.19
(1,597)	1:1529:A:LEU:HD22	1:1529:A:LEU:HA	11	0.19
(1,583)	1:1540:A:ALA:HB1	1:1638:A:PHE:HE1	8	0.19
(1,547)	1:1642:A:THR:HG21	1:1612:A:PHE:HB2	20	0.19
(1,531)	1:1591:A:VAL:HG13	1:1591:A:VAL:HA	16	0.19
(1,494)	1:1610:A:ILE:HG21	1:1638:A:PHE:HD2	4	0.19
(1,465)	1:1625:A:MET:HE2	1:1625:A:MET:H	4	0.19
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	2	0.19
(1,444)	1:1550:A:MET:HE2	1:1610:A:ILE:HA	2	0.19
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	8	0.19
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD12	8	0.19
(1,374)	2:15:B:ASP:H	2:12:B:GLU:HG2	11	0.19
(1,368)	1:1542:A:TYR:HE1	2:19:B:PHE:HA	18	0.19
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	10	0.19
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	6	0.19
(1,339)	2:5:B:SER:H	2:5:B:SER:HB2	7	0.19
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	9	0.19
(1,331)	2:18:B:GLN:H	2:17:B:LEU:HB3	6	0.19
(1,316)	2:58:B:THR:H	2:55:B:LEU:HB3	6	0.19
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD23	8	0.19
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	18	0.19
(1,295)	2:35:B:VAL:H	2:34:B:ARG:HG2	6	0.19
(1,282)	2:46:B:CYS:HA	2:13:B:LEU:HD21	8	0.19
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	6	0.19
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	15	0.19
(1,275)	2:13:B:LEU:HD22	2:8:B:LEU:HA	6	0.19
(1,267)	2:35:B:VAL:HG22	2:37:B:ARG:HD3	19	0.19
(1,266)	2:62:B:THR:HG23	2:63:B:PRO:HG3	3	0.19
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	2	0.19
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	4	0.19
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	15	0.19
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	2	0.19
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	5	0.19
(1,230)	2:55:B:LEU:HD11	2:59:B:TYR:H	4	0.19
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	7	0.19
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	8	0.19
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	8	0.19
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	16	0.19
(1,67)	1:1601:A:LYS:HG2	1:1600:A:SER:HB2	17	0.19
(1,63)	1:1526:A:LEU:HD21	1:1517:A:GLN:HG3	3	0.19
(1,41)	1:1548:A:VAL:HG22	1:1638:A:PHE:HE1	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:1609:A:VAL:HG22	1:1607:A:LYS:HB3	8	0.19
(1,28)	1:1589:A:GLN:HB2	1:1584:A:VAL:HG12	14	0.19
(1,26)	1:1591:A:VAL:HG13	1:1593:A:LYS:HE3	11	0.19
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	12	0.19
(1,21)	1:1645:A:ALA:HB2	1:1612:A:PHE:HA	17	0.19
(1,17)	1:1577:A:ALA:HB2	1:1553:A:CYS:H	6	0.19
(1,14)	1:1552:A:ILE:HG21	1:1529:A:LEU:HD13	6	0.19
(1,9)	1:1550:A:MET:HE1	1:1551:A:SER:H	11	0.19
(1,8)	1:1610:A:ILE:HD12	1:1612:A:PHE:HZ	6	0.19
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	2	0.19
(1,2)	1:1552:A:ILE:HD11	1:1592:A:TYR:HD2	5	0.19
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	13	0.18
(1,3019)	2:18:B:GLN:HG3	1:1545:A:SER:HB3	20	0.18
(1,3013)	1:1629:A:LEU:HD12	2:19:B:PHE:HZ	7	0.18
(1,2994)	2:17:B:LEU:H	2:17:B:LEU:HD12	13	0.18
(1,2989)	2:46:B:CYS:HA	2:13:B:LEU:HD22	5	0.18
(1,2957)	2:28:B:PHE:HD2	2:14:B:VAL:HG21	1	0.18
(1,2947)	2:19:B:PHE:HD1	2:20:B:VAL:HA	9	0.18
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	9	0.18
(1,2935)	2:50:B:SER:H	2:49:B:ARG:HB3	16	0.18
(1,2928)	2:59:B:TYR:H	2:59:B:TYR:HB3	6	0.18
(1,2838)	2:33:B:SER:H	2:32:B:ALA:HB2	20	0.18
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	10	0.18
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG23	9	0.18
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	11	0.18
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	11	0.18
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD11	15	0.18
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD1	1	0.18
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	20	0.18
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD22	2	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	4	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	10	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	11	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	13	0.18
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	15	0.18
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB3	12	0.18
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	4	0.18
(1,2685)	2:6:B:GLU:H	2:5:B:SER:HA	8	0.18
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG21	13	0.18
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	8	0.18
(1,2643)	2:41:B:GLY:H	2:40:B:ARG:HA	3	0.18
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG2	19	0.18
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	1	0.18
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	13	0.18
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	4	0.18
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	10	0.18
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	19	0.18
(1,2521)	2:35:B:VAL:HG21	2:33:B:SER:HB3	11	0.18
(1,2501)	2:56:B:LEU:HD11	2:20:B:VAL:HG11	13	0.18
(1,2498)	2:63:B:PRO:HG3	2:62:B:THR:HA	14	0.18
(1,2480)	2:13:B:LEU:HD13	2:13:B:LEU:HA	1	0.18
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	9	0.18
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	8	0.18
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	11	0.18
(1,2376)	2:42:B:ILE:HG23	2:28:B:PHE:HB3	16	0.18
(1,2373)	2:42:B:ILE:HG23	2:59:B:TYR:HD1	16	0.18
(1,2339)	2:18:B:GLN:HG3	2:26:B:PHE:HD1	16	0.18
(1,2330)	2:61:B:ALA:HB2	2:60:B:CYS:HA	9	0.18
(1,2327)	2:65:B:LYS:H	2:64:B:ALA:HB2	16	0.18
(1,2323)	2:32:B:ALA:HB3	2:33:B:SER:HB2	8	0.18
(1,2303)	2:20:B:VAL:HG21	2:19:B:PHE:HE2	6	0.18
(1,2286)	2:42:B:ILE:HD11	2:28:B:PHE:HD2	6	0.18
(1,2245)	1:1592:A:TYR:HH	1:1590:A:LEU:HD22	17	0.18
(1,2147)	1:1591:A:VAL:HG21	1:1610:A:ILE:H	2	0.18
(1,2147)	1:1591:A:VAL:HG21	1:1610:A:ILE:H	15	0.18
(1,2135)	1:1637:A:PHE:H	1:1627:A:ILE:HG12	9	0.18
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	19	0.18
(1,2038)	1:1567:A:PHE:H	1:1567:A:PHE:HE2	15	0.18
(1,2012)	1:1555:A:GLU:HG2	1:1555:A:GLU:H	3	0.18
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	1	0.18
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	5	0.18
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	3	0.18
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	11	0.18
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	14	0.18
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	15	0.18
(1,1965)	1:1568:A:GLY:H	1:1549:A:TYR:HE2	14	0.18
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	19	0.18
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	5	0.18
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD21	1	0.18
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	2	0.18
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	19	0.18
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	16	0.18
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG12	12	0.18
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	4	0.18
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	5	0.18
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	8	0.18
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	3	0.18
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	18	0.18
(1,1456)	1:1514:A:ASP:HB3	1:1514:A:ASP:H	4	0.18
(1,1331)	1:1569:A:GLN:HG2	1:1569:A:GLN:H	16	0.18
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	9	0.18
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	16	0.18
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	6	0.18
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	4	0.18
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	15	0.18
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	17	0.18
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG21	20	0.18
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	10	0.18
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	2	0.18
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	5	0.18
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	18	0.18
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	16	0.18
(1,1115)	1:1529:A:LEU:HD21	1:1581:A:LEU:HA	16	0.18
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	16	0.18
(1,1092)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	12	0.18
(1,1075)	1:1581:A:LEU:HD22	1:1590:A:LEU:HD11	16	0.18
(1,1029)	1:1610:A:ILE:HG22	1:1640:A:TRP:HZ3	9	0.18
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	5	0.18
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	15	0.18
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG22	16	0.18
(1,1005)	1:1532:A:LEU:HD23	1:1612:A:PHE:HZ	13	0.18
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	12	0.18
(1,992)	1:1610:A:ILE:HD12	1:1610:A:ILE:HA	17	0.18
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	20	0.18
(1,991)	1:1618:A:ALA:HB2	1:1617:A:GLU:HA	1	0.18
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	20	0.18
(1,959)	1:1610:A:ILE:HD13	1:1611:A:SER:H	9	0.18
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	2	0.18
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	3	0.18
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	7	0.18
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	19	0.18
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE2	13	0.18
(1,890)	1:1544:A:LYS:HA	1:1544:A:LYS:HG3	13	0.18
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	20	0.18
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	12	0.18
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	12	0.18
(1,828)	1:1549:A:TYR:HB2	1:1547:A:VAL:HG23	15	0.18
(1,823)	1:1623:A:ARG:HD2	1:1623:A:ARG:HE	16	0.18
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	4	0.18
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG22	13	0.18
(1,775)	1:1632:A:GLN:HG2	1:1633:A:THR:HG22	8	0.18
(1,763)	1:1625:A:MET:HG3	1:1625:A:MET:H	4	0.18
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	1	0.18
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	9	0.18
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	10	0.18
(1,748)	1:1513:A:HIS:HB3	1:1512:A:GLU:HA	19	0.18
(1,731)	1:1626:A:LEU:HD13	1:1626:A:LEU:H	9	0.18
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	20	0.18
(1,722)	1:1581:A:LEU:HD12	1:1518:A:VAL:HB	19	0.18
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	11	0.18
(1,680)	1:1529:A:LEU:HD13	1:1588:A:LEU:HD12	20	0.18
(1,677)	1:1529:A:LEU:HD11	1:1590:A:LEU:HD13	18	0.18
(1,619)	1:1626:A:LEU:HD23	1:1629:A:LEU:HD12	15	0.18
(1,614)	1:1626:A:LEU:HD22	1:1636:A:LEU:HB2	2	0.18
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	7	0.18
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	19	0.18
(1,599)	1:1587:A:VAL:HG12	1:1611:A:SER:HB2	3	0.18
(1,583)	1:1540:A:ALA:HB3	1:1638:A:PHE:HE1	19	0.18
(1,553)	1:1541:A:ALA:HB1	1:1540:A:ALA:HA	19	0.18
(1,536)	1:1609:A:VAL:HG21	1:1607:A:LYS:HE3	14	0.18
(1,510)	1:1645:A:ALA:HB3	1:1612:A:PHE:HD1	19	0.18
(1,509)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD21	16	0.18
(1,479)	1:1552:A:ILE:HG22	1:1529:A:LEU:HB3	3	0.18
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	12	0.18
(1,467)	1:1625:A:MET:HE2	1:1625:A:MET:HA	13	0.18
(1,465)	1:1625:A:MET:HE3	1:1625:A:MET:H	1	0.18
(1,456)	1:1572:A:ILE:HD13	1:1572:A:ILE:HB	9	0.18
(1,440)	1:1550:A:MET:HE3	1:1638:A:PHE:HD2	17	0.18
(1,424)	1:1552:A:ILE:HD12	1:1592:A:TYR:HH	20	0.18
(1,411)	1:1602:A:SER:H	2:52:B:ASP:HA	2	0.18
(1,411)	1:1602:A:SER:H	2:52:B:ASP:HA	12	0.18
(1,375)	1:1600:A:SER:H	2:53:B:LEU:HD13	11	0.18
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	14	0.18
(1,353)	2:61:B:ALA:HB3	2:60:B:CYS:HB2	2	0.18
(1,340)	2:66:B:SER:HB3	2:66:B:SER:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	2:55:B:LEU:HD13	2:56:B:LEU:H	3	0.18
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG21	19	0.18
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD22	14	0.18
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB1	7	0.18
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	13	0.18
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	19	0.18
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	8	0.18
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	8	0.18
(1,208)	1:1609:A:VAL:HG12	1:1590:A:LEU:H	11	0.18
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	4	0.18
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	11	0.18
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	13	0.18
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD21	6	0.18
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	3	0.18
(1,81)	1:1512:A:GLU:HG2	1:1511:A:ASN:H	12	0.18
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB2	12	0.18
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	15	0.18
(1,15)	1:1577:A:ALA:HB1	1:1555:A:GLU:HG2	16	0.18
(1,13)	1:1547:A:VAL:HG22	1:1548:A:VAL:HA	6	0.18
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	5	0.17
(1,3017)	2:18:B:GLN:HE22	1:1545:A:SER:HB3	15	0.17
(1,3015)	2:19:B:PHE:HE1	1:1636:A:LEU:HD22	6	0.17
(1,3008)	2:56:B:LEU:HD21	2:17:B:LEU:H	9	0.17
(1,2991)	2:42:B:ILE:HG22	2:59:B:TYR:HE2	6	0.17
(1,2987)	2:42:B:ILE:HD12	2:56:B:LEU:HG	19	0.17
(1,2958)	2:61:B:ALA:HB1	2:27:B:TYR:HD2	1	0.17
(1,2928)	2:59:B:TYR:H	2:59:B:TYR:HB3	2	0.17
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	9	0.17
(1,2874)	2:17:B:LEU:HD11	2:28:B:PHE:HD1	17	0.17
(1,2831)	2:41:B:GLY:H	2:42:B:ILE:HG12	3	0.17
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	2	0.17
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG11	16	0.17
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG22	6	0.17
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG22	8	0.17
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	10	0.17
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	13	0.17
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	20	0.17
(1,2681)	2:5:B:SER:H	2:5:B:SER:HB2	14	0.17
(1,2646)	2:41:B:GLY:H	2:42:B:ILE:H	4	0.17
(1,2641)	2:41:B:GLY:H	2:40:B:ARG:HB3	10	0.17
(1,2634)	2:38:B:ARG:H	2:37:B:ARG:HG3	9	0.17
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	12	0.17
(1,2604)	2:34:B:ARG:H	2:33:B:SER:HB2	4	0.17
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	13	0.17
(1,2536)	2:12:B:GLU:H	2:11:B:GLY:HA3	15	0.17
(1,2521)	2:35:B:VAL:HG22	2:33:B:SER:HB3	16	0.17
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	7	0.17
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	11	0.17
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	5	0.17
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB3	10	0.17
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	15	0.17
(1,2375)	2:42:B:ILE:HG23	2:28:B:PHE:HA	1	0.17
(1,2373)	2:42:B:ILE:HG21	2:59:B:TYR:HD2	7	0.17
(1,2330)	2:61:B:ALA:HB1	2:60:B:CYS:HA	1	0.17
(1,2323)	2:32:B:ALA:HB3	2:36:B:SER:HB3	14	0.17
(1,2322)	2:32:B:ALA:HB2	2:33:B:SER:HB3	11	0.17
(1,2292)	2:17:B:LEU:HD11	2:42:B:ILE:HG13	5	0.17
(1,2281)	2:42:B:ILE:HD11	2:59:B:TYR:HB3	8	0.17
(1,2236)	1:1549:A:TYR:HD1	1:1556:A:ASN:HD21	1	0.17
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB1	7	0.17
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB2	7	0.17
(1,2234)	1:1592:A:TYR:HE2	1:1577:A:ALA:HB3	7	0.17
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG12	6	0.17
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG11	18	0.17
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	17	0.17
(1,2079)	1:1588:A:LEU:HD11	1:1583:A:TYR:H	9	0.17
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	13	0.17
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	12	0.17
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	17	0.17
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	9	0.17
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE2	2	0.17
(1,1975)	1:1538:A:PHE:H	1:1538:A:PHE:HD1	17	0.17
(1,1927)	1:1563:A:VAL:HG23	1:1575:A:GLY:H	11	0.17
(1,1919)	1:1619:A:GLY:H	1:1620:A:PRO:HD2	11	0.17
(1,1901)	1:1545:A:SER:H	1:1544:A:LYS:HD2	15	0.17
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG21	7	0.17
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG21	11	0.17
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	10	0.17
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	17	0.17
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD23	18	0.17
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	3	0.17
(1,1625)	1:1509:A:LYS:HA	1:1510:A:SER:H	20	0.17
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:1553:A:CYS:H	1:1592:A:TYR:HH	19	0.17
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	5	0.17
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	8	0.17
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	15	0.17
(1,1501)	1:1528:A:ASP:H	1:1527:A:PHE:HD1	15	0.17
(1,1476)	1:1532:A:LEU:H	1:1532:A:LEU:HD11	2	0.17
(1,1457)	1:1514:A:ASP:HB2	1:1514:A:ASP:H	20	0.17
(1,1405)	1:1539:A:THR:HG22	1:1540:A:ALA:H	10	0.17
(1,1395)	1:1591:A:VAL:H	1:1590:A:LEU:HB3	5	0.17
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	19	0.17
(1,1301)	1:1557:A:GLU:H	1:1558:A:ASN:HD22	15	0.17
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	20	0.17
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	11	0.17
(1,1280)	1:1618:A:ALA:H	1:1617:A:GLU:HB2	2	0.17
(1,1280)	1:1618:A:ALA:H	1:1617:A:GLU:HB2	7	0.17
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	14	0.17
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	2	0.17
(1,1261)	1:1527:A:PHE:H	1:1526:A:LEU:HD12	15	0.17
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD22	4	0.17
(1,1248)	1:1529:A:LEU:H	1:1581:A:LEU:HD23	8	0.17
(1,1228)	1:1642:A:THR:HG21	1:1640:A:TRP:HE1	5	0.17
(1,1228)	1:1642:A:THR:HG21	1:1640:A:TRP:HE1	16	0.17
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	13	0.17
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	6	0.17
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG3	12	0.17
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	17	0.17
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	18	0.17
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	19	0.17
(1,1139)	1:1577:A:ALA:HB2	1:1554:A:GLY:H	1	0.17
(1,1139)	1:1577:A:ALA:HB1	1:1554:A:GLY:H	2	0.17
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	5	0.17
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	17	0.17
(1,1130)	1:1554:A:GLY:H	1:1592:A:TYR:HH	7	0.17
(1,1075)	1:1581:A:LEU:HD23	1:1590:A:LEU:HD12	10	0.17
(1,1072)	1:1590:A:LEU:HD22	1:1553:A:CYS:HA	12	0.17
(1,1040)	1:1591:A:VAL:HG23	1:1607:A:LYS:HD3	7	0.17
(1,1031)	1:1577:A:ALA:HB3	1:1562:A:GLY:HA3	6	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	3	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	4	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	8	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	9	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	13	0.17
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	17	0.17
(1,992)	1:1610:A:ILE:HD13	1:1610:A:ILE:HA	10	0.17
(1,991)	1:1618:A:ALA:HB2	1:1617:A:GLU:HA	15	0.17
(1,987)	1:1627:A:ILE:HD13	1:1638:A:PHE:HA	13	0.17
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	8	0.17
(1,955)	1:1574:A:VAL:HG11	1:1567:A:PHE:HD1	14	0.17
(1,917)	1:1572:A:ILE:HA	1:1572:A:ILE:HG12	17	0.17
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	8	0.17
(1,794)	1:1617:A:GLU:HG3	1:1618:A:ALA:H	1	0.17
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	12	0.17
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	19	0.17
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD13	5	0.17
(1,691)	1:1644:A:LEU:HD23	1:1527:A:PHE:HE1	1	0.17
(1,668)	1:1635:A:THR:HG21	1:1607:A:LYS:HG3	19	0.17
(1,646)	1:1529:A:LEU:HD11	1:1612:A:PHE:HZ	2	0.17
(1,646)	1:1529:A:LEU:HD11	1:1612:A:PHE:HZ	3	0.17
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	10	0.17
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	3	0.17
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	4	0.17
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	18	0.17
(1,597)	1:1529:A:LEU:HD23	1:1529:A:LEU:HA	5	0.17
(1,596)	1:1529:A:LEU:HD22	1:1645:A:ALA:HA	19	0.17
(1,553)	1:1541:A:ALA:HB2	1:1540:A:ALA:HA	15	0.17
(1,549)	1:1574:A:VAL:HG21	1:1636:A:LEU:HB2	14	0.17
(1,524)	1:1577:A:ALA:HB2	1:1592:A:TYR:HE2	15	0.17
(1,504)	1:1618:A:ALA:HB2	1:1619:A:GLY:HA2	1	0.17
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	3	0.17
(1,478)	1:1552:A:ILE:HG22	1:1552:A:ILE:HG12	4	0.17
(1,458)	1:1572:A:ILE:HD12	1:1572:A:ILE:H	7	0.17
(1,457)	1:1550:A:MET:HE1	1:1550:A:MET:HA	9	0.17
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	12	0.17
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	13	0.17
(1,443)	1:1550:A:MET:HE1	1:1550:A:MET:H	14	0.17
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG13	2	0.17
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB2	6	0.17
(1,373)	2:18:B:GLN:HE21	1:1570:A:THR:HG23	16	0.17
(1,371)	2:18:B:GLN:HG2	2:26:B:PHE:HD2	17	0.17
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	17	0.17
(1,339)	2:5:B:SER:H	2:5:B:SER:HB2	16	0.17
(1,332)	2:55:B:LEU:HD11	2:42:B:ILE:H	13	0.17
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	2:17:B:LEU:HD12	2:27:B:TYR:HD1	9	0.17
(1,271)	2:54:B:ALA:HB3	2:53:B:LEU:HD13	16	0.17
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	15	0.17
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD23	16	0.17
(1,226)	2:17:B:LEU:HD12	2:57:B:GLU:HA	2	0.17
(1,183)	1:1608:A:SER:H	1:1609:A:VAL:HG23	12	0.17
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	18	0.17
(1,149)	1:1638:A:PHE:HD2	1:1636:A:LEU:HD21	8	0.17
(1,144)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	1	0.17
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	12	0.17
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	20	0.17
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	6	0.17
(1,53)	1:1588:A:LEU:HD12	1:1583:A:TYR:H	16	0.17
(1,32)	1:1547:A:VAL:HG21	1:1549:A:TYR:HB3	5	0.17
(1,13)	1:1547:A:VAL:HG22	1:1548:A:VAL:HA	3	0.17
(1,6)	1:1552:A:ILE:HD11	1:1532:A:LEU:HB2	12	0.17
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	14	0.17
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	17	0.17
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD22	1	0.16
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	4	0.16
(1,3008)	2:56:B:LEU:HD21	2:17:B:LEU:H	6	0.16
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	17	0.16
(1,2922)	2:61:B:ALA:HA	2:27:B:TYR:HD1	20	0.16
(1,2850)	2:13:B:LEU:H	2:13:B:LEU:HD23	13	0.16
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	10	0.16
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	5	0.16
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	6	0.16
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG13	7	0.16
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	7	0.16
(1,2806)	2:22:B:GLY:H	2:20:B:VAL:HG23	18	0.16
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG21	16	0.16
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	2	0.16
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	9	0.16
(1,2795)	2:53:B:LEU:H	2:53:B:LEU:HB3	14	0.16
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD1	13	0.16
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	16	0.16
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	12	0.16
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	7	0.16
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG23	14	0.16
(1,2659)	2:64:B:ALA:H	2:62:B:THR:HG21	17	0.16
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	17	0.16
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	11	0.16
(1,2581)	2:32:B:ALA:H	2:32:B:ALA:HB1	4	0.16
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD3	6	0.16
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	8	0.16
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	9	0.16
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	12	0.16
(1,2549)	2:7:B:THR:H	2:6:B:GLU:HG3	19	0.16
(1,2531)	2:61:B:ALA:HB3	2:62:B:THR:HA	14	0.16
(1,2515)	2:55:B:LEU:HD22	2:46:B:CYS:HA	12	0.16
(1,2499)	2:56:B:LEU:HD11	2:20:B:VAL:HB	12	0.16
(1,2471)	2:37:B:ARG:HG3	2:38:B:ARG:H	14	0.16
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	11	0.16
(1,2423)	2:18:B:GLN:HB3	2:18:B:GLN:HG2	7	0.16
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	4	0.16
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	5	0.16
(1,2382)	2:55:B:LEU:HD23	2:51:B:CYS:HA	1	0.16
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	5	0.16
(1,2292)	2:17:B:LEU:HD13	2:42:B:ILE:HG13	8	0.16
(1,2249)	2:28:B:PHE:HD2	2:43:B:VAL:HG22	13	0.16
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG23	11	0.16
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD2	13	0.16
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	19	0.16
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	13	0.16
(1,1911)	1:1589:A:GLN:HE22	1:1584:A:VAL:HG13	20	0.16
(1,1901)	1:1545:A:SER:H	1:1544:A:LYS:HD2	1	0.16
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	8	0.16
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG12	3	0.16
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	19	0.16
(1,1712)	1:1572:A:ILE:HG23	1:1596:A:SER:H	11	0.16
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	6	0.16
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG21	9	0.16
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	13	0.16
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	3	0.16
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	12	0.16
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	17	0.16
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD13	14	0.16
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	20	0.16
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	4	0.16
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	12	0.16
(1,1494)	1:1510:A:SER:HB3	1:1511:A:ASN:H	16	0.16
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG22	14	0.16
(1,1395)	1:1591:A:VAL:H	1:1590:A:LEU:HB3	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	8	0.16
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG12	14	0.16
(1,1349)	1:1582:A:ARG:H	1:1582:A:ARG:HG2	12	0.16
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	12	0.16
(1,1287)	1:1635:A:THR:HG22	1:1609:A:VAL:H	3	0.16
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	7	0.16
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG23	20	0.16
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	8	0.16
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	19	0.16
(1,1085)	1:1636:A:LEU:HD12	1:1574:A:VAL:HG22	16	0.16
(1,1054)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	12	0.16
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	18	0.16
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG22	20	0.16
(1,1005)	1:1532:A:LEU:HD21	1:1612:A:PHE:HD1	8	0.16
(1,992)	1:1610:A:ILE:HD11	1:1610:A:ILE:HA	3	0.16
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	4	0.16
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	1	0.16
(1,974)	1:1533:A:SER:HB3	1:1552:A:ILE:HB	3	0.16
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	16	0.16
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	18	0.16
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	5	0.16
(1,865)	1:1581:A:LEU:HA	1:1581:A:LEU:HD21	1	0.16
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	9	0.16
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	11	0.16
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	15	0.16
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	15	0.16
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	1	0.16
(1,835)	1:1590:A:LEU:HB2	1:1590:A:LEU:H	16	0.16
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	10	0.16
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	16	0.16
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG21	15	0.16
(1,794)	1:1617:A:GLU:HG2	1:1618:A:ALA:H	6	0.16
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG22	3	0.16
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	3	0.16
(1,724)	1:1581:A:LEU:HD21	1:1588:A:LEU:HA	10	0.16
(1,646)	1:1529:A:LEU:HD12	1:1612:A:PHE:HZ	7	0.16
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	8	0.16
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	9	0.16
(1,646)	1:1529:A:LEU:HD13	1:1612:A:PHE:HZ	13	0.16
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	11	0.16
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	20	0.16
(1,598)	1:1587:A:VAL:HG23	1:1613:A:VAL:HA	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:1635:A:THR:HG21	1:1637:A:PHE:HA	13	0.16
(1,581)	1:1532:A:LEU:HD21	1:1532:A:LEU:H	6	0.16
(1,504)	1:1618:A:ALA:HB2	1:1619:A:GLY:HA2	12	0.16
(1,467)	1:1625:A:MET:HE3	1:1625:A:MET:HA	2	0.16
(1,467)	1:1625:A:MET:HE2	1:1625:A:MET:HA	6	0.16
(1,467)	1:1625:A:MET:HE3	1:1625:A:MET:HA	12	0.16
(1,458)	1:1572:A:ILE:HD11	1:1572:A:ILE:H	14	0.16
(1,451)	1:1550:A:MET:HE2	1:1610:A:ILE:HG13	1	0.16
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	7	0.16
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	10	0.16
(1,422)	1:1627:A:ILE:HD12	1:1627:A:ILE:HB	15	0.16
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG11	20	0.16
(1,381)	2:12:B:GLU:HG3	1:1570:A:THR:HB	18	0.16
(1,376)	2:54:B:ALA:HB1	2:52:B:ASP:H	14	0.16
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	8	0.16
(1,326)	2:6:B:GLU:H	2:7:B:THR:HG21	9	0.16
(1,323)	2:60:B:CYS:H	2:42:B:ILE:HG22	2	0.16
(1,312)	2:46:B:CYS:H	2:49:B:ARG:HB3	19	0.16
(1,304)	2:54:B:ALA:H	2:53:B:LEU:HD21	4	0.16
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG2	17	0.16
(1,277)	2:56:B:LEU:HD11	2:53:B:LEU:H	17	0.16
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	2	0.16
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	5	0.16
(1,235)	2:20:B:VAL:HG13	2:57:B:GLU:HA	2	0.16
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	11	0.16
(1,210)	1:1517:A:GLN:HE22	1:1515:A:ASP:HB3	12	0.16
(1,187)	1:1567:A:PHE:H	1:1548:A:VAL:HG23	15	0.16
(1,172)	1:1513:A:HIS:H	1:1514:A:ASP:HB2	20	0.16
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	12	0.16
(1,149)	1:1638:A:PHE:HD1	1:1540:A:ALA:HB2	19	0.16
(1,142)	1:1581:A:LEU:HD11	1:1582:A:ARG:HG3	9	0.16
(1,97)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	1	0.16
(1,97)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	8	0.16
(1,74)	1:1579:A:LYS:HD2	1:1578:A:ASN:HA	7	0.16
(1,61)	1:1526:A:LEU:HD22	1:1528:A:ASP:HB2	15	0.16
(1,59)	1:1590:A:LEU:HD21	1:1578:A:ASN:HB2	12	0.16
(1,59)	1:1590:A:LEU:HD23	1:1578:A:ASN:HB2	19	0.16
(1,53)	1:1588:A:LEU:HD11	1:1583:A:TYR:H	10	0.16
(1,46)	1:1540:A:ALA:HB1	1:1541:A:ALA:HA	13	0.16
(1,32)	1:1547:A:VAL:HG23	1:1567:A:PHE:HB3	4	0.16
(1,17)	1:1577:A:ALA:HB1	1:1553:A:CYS:H	4	0.16
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:1552:A:ILE:HG23	1:1529:A:LEU:HD13	11	0.16
(1,11)	1:1625:A:MET:HE3	1:1624:A:PRO:HA	3	0.16
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	14	0.15
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE1	4	0.15
(1,2957)	2:28:B:PHE:HD1	2:14:B:VAL:HG23	8	0.15
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	4	0.15
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	19	0.15
(1,2861)	2:20:B:VAL:HG22	2:19:B:PHE:HD2	7	0.15
(1,2843)	2:60:B:CYS:H	2:17:B:LEU:HD21	12	0.15
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	15	0.15
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	18	0.15
(1,2801)	2:47:B:CYS:H	2:43:B:VAL:HG23	11	0.15
(1,2799)	2:9:B:CYS:H	2:10:B:GLY:H	16	0.15
(1,2797)	2:62:B:THR:H	2:24:B:ARG:HG2	20	0.15
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	7	0.15
(1,2788)	2:32:B:ALA:H	2:33:B:SER:HA	14	0.15
(1,2770)	2:66:B:SER:H	2:65:B:LYS:HD2	16	0.15
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	18	0.15
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB1	16	0.15
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	10	0.15
(1,2640)	2:41:B:GLY:H	2:40:B:ARG:HB2	14	0.15
(1,2636)	2:38:B:ARG:H	2:38:B:ARG:HD2	4	0.15
(1,2621)	2:37:B:ARG:H	2:37:B:ARG:HD2	15	0.15
(1,2604)	2:34:B:ARG:H	2:33:B:SER:HB2	12	0.15
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	7	0.15
(1,2581)	2:32:B:ALA:H	2:32:B:ALA:HB2	14	0.15
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG23	1	0.15
(1,2524)	2:64:B:ALA:HA	2:65:B:LYS:HB2	18	0.15
(1,2514)	2:13:B:LEU:HD22	2:13:B:LEU:HA	5	0.15
(1,2481)	2:13:B:LEU:HD13	2:14:B:VAL:HB	7	0.15
(1,2479)	2:35:B:VAL:HG22	2:34:B:ARG:HA	13	0.15
(1,2454)	2:35:B:VAL:HG23	2:34:B:ARG:HA	17	0.15
(1,2430)	2:63:B:PRO:HD2	2:63:B:PRO:HB3	10	0.15
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	9	0.15
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	12	0.15
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	15	0.15
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	17	0.15
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	18	0.15
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	19	0.15
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	12	0.15
(1,2376)	2:42:B:ILE:HG22	2:28:B:PHE:HB3	9	0.15
(1,2373)	2:42:B:ILE:HG22	2:59:B:TYR:HD1	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	2:27:B:TYR:HE2	2:27:B:TYR:HB3	14	0.15
(1,2322)	2:32:B:ALA:HB1	2:33:B:SER:HB3	1	0.15
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE1	2	0.15
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	18	0.15
(1,2297)	2:52:B:ASP:H	2:55:B:LEU:HD21	14	0.15
(1,2295)	2:17:B:LEU:HD22	2:56:B:LEU:HA	19	0.15
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	2	0.15
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG21	2	0.15
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG13	10	0.15
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	9	0.15
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	11	0.15
(1,2158)	1:1530:A:SER:H	1:1644:A:LEU:HD11	13	0.15
(1,2147)	1:1591:A:VAL:HG22	1:1610:A:ILE:H	7	0.15
(1,2053)	1:1573:A:SER:H	1:1563:A:VAL:HG21	5	0.15
(1,2049)	1:1572:A:ILE:H	1:1566:A:CYS:HB2	14	0.15
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	4	0.15
(1,1983)	1:1537:A:GLY:H	1:1538:A:PHE:HE1	20	0.15
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	13	0.15
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	12	0.15
(1,1837)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD22	20	0.15
(1,1770)	1:1547:A:VAL:H	1:1549:A:TYR:HE2	15	0.15
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	15	0.15
(1,1694)	1:1645:A:ALA:H	1:1644:A:LEU:HB3	7	0.15
(1,1694)	1:1645:A:ALA:H	1:1644:A:LEU:HB3	19	0.15
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG22	4	0.15
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	4	0.15
(1,1633)	1:1616:A:PRO:HB2	1:1617:A:GLU:H	13	0.15
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	7	0.15
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	10	0.15
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	11	0.15
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	14	0.15
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	18	0.15
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	15	0.15
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	12	0.15
(1,1450)	1:1589:A:GLN:H	1:1581:A:LEU:HD12	17	0.15
(1,1405)	1:1539:A:THR:HG23	1:1540:A:ALA:H	9	0.15
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	14	0.15
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	15	0.15
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	19	0.15
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	1	0.15
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	12	0.15
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	4	0.15
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	11	0.15
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	3	0.15
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	8	0.15
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	6	0.15
(1,1180)	1:1610:A:ILE:HD13	1:1610:A:ILE:H	16	0.15
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	8	0.15
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	10	0.15
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	20	0.15
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	3	0.15
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG23	2	0.15
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG21	7	0.15
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	10	0.15
(1,1088)	1:1636:A:LEU:HD21	1:1606:A:TYR:HE1	13	0.15
(1,1085)	1:1636:A:LEU:HD12	1:1574:A:VAL:HG22	3	0.15
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	20	0.15
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	8	0.15
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	10	0.15
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG22	14	0.15
(1,1018)	1:1527:A:PHE:HE2	1:1518:A:VAL:HG21	18	0.15
(1,991)	1:1618:A:ALA:HB3	1:1617:A:GLU:HA	12	0.15
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	20	0.15
(1,983)	1:1580:A:ARG:HD3	1:1580:A:ARG:HA	19	0.15
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	12	0.15
(1,941)	1:1539:A:THR:HA	1:1547:A:VAL:HG13	8	0.15
(1,932)	1:1601:A:LYS:HD2	1:1604:A:LEU:HD21	7	0.15
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	17	0.15
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	10	0.15
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	10	0.15
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	18	0.15
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	18	0.15
(1,832)	1:1581:A:LEU:HD23	1:1590:A:LEU:HB2	7	0.15
(1,832)	1:1581:A:LEU:HD23	1:1590:A:LEU:HB2	17	0.15
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	2	0.15
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	4	0.15
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	16	0.15
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	17	0.15
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG22	17	0.15
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	2	0.15
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	18	0.15
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	9	0.15
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD11	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:1581:A:LEU:HD11	1:1518:A:VAL:H	3	0.15
(1,705)	1:1581:A:LEU:HD12	1:1518:A:VAL:H	19	0.15
(1,654)	1:1590:A:LEU:HD22	1:1592:A:TYR:HD1	5	0.15
(1,638)	1:1588:A:LEU:HD21	1:1588:A:LEU:HB2	14	0.15
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	9	0.15
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	13	0.15
(1,605)	1:1518:A:VAL:HG11	1:1518:A:VAL:HB	14	0.15
(1,599)	1:1587:A:VAL:HG12	1:1611:A:SER:HB2	15	0.15
(1,597)	1:1529:A:LEU:HD21	1:1529:A:LEU:HA	19	0.15
(1,483)	1:1610:A:ILE:HG23	1:1590:A:LEU:HB3	2	0.15
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	1	0.15
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	2	0.15
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	17	0.15
(1,478)	1:1552:A:ILE:HG22	1:1552:A:ILE:HG12	18	0.15
(1,458)	1:1572:A:ILE:HD13	1:1572:A:ILE:H	13	0.15
(1,443)	1:1550:A:MET:HE1	1:1550:A:MET:H	11	0.15
(1,439)	1:1550:A:MET:HE1	1:1638:A:PHE:HE1	13	0.15
(1,424)	1:1552:A:ILE:HD11	1:1592:A:TYR:HH	19	0.15
(1,420)	1:1627:A:ILE:HD11	1:1639:A:SER:HB2	17	0.15
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD12	3	0.15
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	9	0.15
(1,332)	2:55:B:LEU:HD13	2:42:B:ILE:H	16	0.15
(1,317)	2:53:B:LEU:H	2:55:B:LEU:HB3	7	0.15
(1,287)	2:64:B:ALA:HA	2:65:B:LYS:HB3	9	0.15
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	17	0.15
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	7	0.15
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG11	15	0.15
(1,208)	1:1609:A:VAL:HG12	1:1590:A:LEU:H	19	0.15
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD22	17	0.15
(1,187)	1:1567:A:PHE:H	1:1548:A:VAL:HG22	8	0.15
(1,142)	1:1581:A:LEU:HD11	1:1582:A:ARG:HG3	13	0.15
(1,103)	1:1610:A:ILE:HD12	1:1590:A:LEU:H	11	0.15
(1,31)	1:1548:A:VAL:HG23	1:1550:A:MET:HG2	6	0.15
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	19	0.15
(1,13)	1:1547:A:VAL:HG22	1:1548:A:VAL:HA	12	0.15
(1,6)	1:1552:A:ILE:HD13	1:1610:A:ILE:HB	15	0.15
(1,2)	1:1552:A:ILE:HD12	1:1592:A:TYR:HD2	20	0.15
(1,3009)	2:56:B:LEU:HD22	2:17:B:LEU:HD23	12	0.14
(1,2991)	2:42:B:ILE:HG23	2:59:B:TYR:HE1	15	0.14
(1,2962)	2:18:B:GLN:HG2	2:26:B:PHE:HE2	7	0.14
(1,2962)	2:18:B:GLN:HG2	2:26:B:PHE:HE2	18	0.14
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	15	0.14
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB3	10	0.14
(1,2815)	2:57:B:GLU:H	2:54:B:ALA:HB2	13	0.14
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	17	0.14
(1,2772)	2:66:B:SER:H	2:65:B:LYS:HA	13	0.14
(1,2747)	2:18:B:GLN:H	2:14:B:VAL:HG22	2	0.14
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD2	6	0.14
(1,2710)	2:49:B:ARG:H	2:49:B:ARG:HB2	5	0.14
(1,2700)	2:3:B:ARG:H	2:3:B:ARG:HG2	18	0.14
(1,2699)	2:3:B:ARG:H	2:3:B:ARG:HB3	18	0.14
(1,2694)	2:2:B:TYR:H	2:1:B:ALA:HB1	3	0.14
(1,2630)	2:36:B:SER:H	2:37:B:ARG:HB3	2	0.14
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	20	0.14
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	8	0.14
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	18	0.14
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	19	0.14
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	13	0.14
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	1	0.14
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	14	0.14
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	17	0.14
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	18	0.14
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG21	20	0.14
(1,2532)	2:56:B:LEU:HA	2:42:B:ILE:HG21	7	0.14
(1,2521)	2:35:B:VAL:HG22	2:33:B:SER:HB3	13	0.14
(1,2515)	2:55:B:LEU:HD23	2:46:B:CYS:HA	20	0.14
(1,2441)	2:8:B:LEU:HD12	2:8:B:LEU:HA	9	0.14
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	13	0.14
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	7	0.14
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	19	0.14
(1,2407)	2:38:B:ARG:HA	2:38:B:ARG:HD3	18	0.14
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG12	16	0.14
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	20	0.14
(1,2376)	2:42:B:ILE:HG21	2:28:B:PHE:HB3	8	0.14
(1,2373)	2:42:B:ILE:HG23	2:59:B:TYR:HD1	13	0.14
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	14	0.14
(1,2323)	2:32:B:ALA:HB3	2:33:B:SER:HB2	5	0.14
(1,2318)	2:33:B:SER:H	2:32:B:ALA:HA	3	0.14
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	3	0.14
(1,2274)	2:14:B:VAL:HG23	2:18:B:GLN:HG3	15	0.14
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG23	10	0.14
(1,2245)	1:1592:A:TYR:HH	1:1590:A:LEU:HD21	12	0.14
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:1530:A:SER:H	1:1516:A:CYS:HB2	8	0.14
(1,2157)	1:1530:A:SER:H	1:1644:A:LEU:HD22	1	0.14
(1,2150)	1:1631:A:LYS:H	1:1631:A:LYS:HG2	4	0.14
(1,2147)	1:1591:A:VAL:HG23	1:1610:A:ILE:H	10	0.14
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	1	0.14
(1,2049)	1:1572:A:ILE:H	1:1571:A:ARG:HD2	12	0.14
(1,2029)	1:1563:A:VAL:H	1:1561:A:PRO:HB3	9	0.14
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	8	0.14
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	18	0.14
(1,1965)	1:1568:A:GLY:H	1:1549:A:TYR:HE2	5	0.14
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	10	0.14
(1,1955)	1:1595:A:GLY:H	1:1576:A:LYS:HB3	8	0.14
(1,1937)	1:1568:A:GLY:H	1:1567:A:PHE:HB3	18	0.14
(1,1925)	1:1575:A:GLY:H	1:1595:A:GLY:HA2	1	0.14
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	3	0.14
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	16	0.14
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	11	0.14
(1,1803)	1:1511:A:ASN:HD21	1:1518:A:VAL:HG11	13	0.14
(1,1709)	1:1632:A:GLN:HB3	1:1632:A:GLN:H	19	0.14
(1,1690)	1:1571:A:ARG:H	1:1571:A:ARG:HD2	1	0.14
(1,1685)	1:1634:A:CYS:H	1:1604:A:LEU:HD23	20	0.14
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG21	7	0.14
(1,1684)	1:1634:A:CYS:H	1:1633:A:THR:HG23	11	0.14
(1,1668)	1:1608:A:SER:H	1:1607:A:LYS:HB2	5	0.14
(1,1624)	1:1510:A:SER:HB2	1:1510:A:SER:H	10	0.14
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD23	19	0.14
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	7	0.14
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	13	0.14
(1,1513)	1:1513:A:HIS:H	1:1512:A:GLU:HG2	18	0.14
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	13	0.14
(1,1450)	1:1589:A:GLN:H	1:1581:A:LEU:HD11	6	0.14
(1,1439)	1:1611:A:SER:HB2	1:1611:A:SER:H	6	0.14
(1,1406)	1:1540:A:ALA:H	1:1547:A:VAL:HG21	8	0.14
(1,1405)	1:1539:A:THR:HG23	1:1540:A:ALA:H	4	0.14
(1,1383)	1:1647:A:GLU:HG3	1:1647:A:GLU:H	17	0.14
(1,1377)	1:1580:A:ARG:H	1:1579:A:LYS:H	2	0.14
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG23	7	0.14
(1,1353)	1:1581:A:LEU:HG	1:1582:A:ARG:H	1	0.14
(1,1322)	1:1577:A:ALA:H	1:1576:A:LYS:HG3	1	0.14
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	2	0.14
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	10	0.14
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	19	0.14
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	20	0.14
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	14	0.14
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG22	9	0.14
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	10	0.14
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG23	12	0.14
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	9	0.14
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	11	0.14
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	15	0.14
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	19	0.14
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG23	16	0.14
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	6	0.14
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	9	0.14
(1,1203)	1:1588:A:LEU:HD23	1:1584:A:VAL:H	16	0.14
(1,1203)	1:1588:A:LEU:HD21	1:1584:A:VAL:H	19	0.14
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	4	0.14
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	2	0.14
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	7	0.14
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	9	0.14
(1,1137)	1:1590:A:LEU:HD13	1:1554:A:GLY:H	1	0.14
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	13	0.14
(1,1112)	1:1641:A:HIS:HD2	1:1613:A:VAL:HG13	14	0.14
(1,1110)	1:1583:A:TYR:HD1	1:1584:A:VAL:HG23	7	0.14
(1,1088)	1:1636:A:LEU:HD22	1:1606:A:TYR:HE1	19	0.14
(1,1076)	1:1526:A:LEU:HD11	1:1528:A:ASP:HB3	17	0.14
(1,1061)	1:1563:A:VAL:HG12	1:1566:A:CYS:HB3	15	0.14
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	19	0.14
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	20	0.14
(1,1033)	1:1645:A:ALA:HB3	1:1614:A:CYS:HB3	16	0.14
(1,1029)	1:1610:A:ILE:HG22	1:1640:A:TRP:HZ3	12	0.14
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	2	0.14
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	7	0.14
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	12	0.14
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG21	14	0.14
(1,1027)	1:1610:A:ILE:HG13	1:1610:A:ILE:HG23	19	0.14
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	20	0.14
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	4	0.14
(1,970)	1:1593:A:LYS:HE3	1:1578:A:ASN:HD21	12	0.14
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	12	0.14
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD2	17	0.14
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD3	17	0.14
(1,860)	1:1647:A:GLU:HG3	1:1647:A:GLU:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1647:A:GLU:HA	1:1648:A:PRO:HD3	5	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	1	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	1	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	3	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	3	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	4	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	4	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	6	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	6	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	11	0.14
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	11	0.14
(1,834)	1:1590:A:LEU:HB2	1:1590:A:LEU:HA	1	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	1	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	3	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	5	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	6	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	7	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	8	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	9	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	10	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	11	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	12	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	13	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	14	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	15	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	18	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	19	0.14
(1,829)	1:1534:A:GLY:HA2	1:1534:A:GLY:HA3	20	0.14
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	6	0.14
(1,823)	1:1623:A:ARG:HD2	1:1623:A:ARG:HE	10	0.14
(1,787)	1:1617:A:GLU:HG2	1:1617:A:GLU:HA	2	0.14
(1,784)	1:1647:A:GLU:HG2	1:1647:A:GLU:HA	7	0.14
(1,782)	1:1569:A:GLN:HG2	1:1570:A:THR:H	16	0.14
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	19	0.14
(1,751)	1:1635:A:THR:HG23	1:1607:A:LYS:HD3	7	0.14
(1,751)	1:1635:A:THR:HG22	1:1607:A:LYS:HD3	8	0.14
(1,731)	1:1626:A:LEU:HD11	1:1626:A:LEU:H	7	0.14
(1,731)	1:1626:A:LEU:HD12	1:1626:A:LEU:H	15	0.14
(1,706)	1:1604:A:LEU:H	1:1604:A:LEU:HD13	14	0.14
(1,650)	1:1590:A:LEU:HD23	1:1581:A:LEU:H	12	0.14
(1,638)	1:1588:A:LEU:HD21	1:1588:A:LEU:HB2	3	0.14
(1,638)	1:1588:A:LEU:HD22	1:1588:A:LEU:HB2	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	6	0.14
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	20	0.14
(1,599)	1:1587:A:VAL:HG13	1:1611:A:SER:HB2	17	0.14
(1,589)	1:1635:A:THR:HG22	1:1637:A:PHE:HA	15	0.14
(1,582)	1:1540:A:ALA:HB1	1:1548:A:VAL:H	8	0.14
(1,581)	1:1532:A:LEU:HD23	1:1532:A:LEU:H	20	0.14
(1,512)	1:1645:A:ALA:HB2	1:1614:A:CYS:H	11	0.14
(1,494)	1:1610:A:ILE:HG23	1:1638:A:PHE:HD2	15	0.14
(1,478)	1:1552:A:ILE:HG22	1:1552:A:ILE:HG12	7	0.14
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	10	0.14
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	13	0.14
(1,478)	1:1552:A:ILE:HG22	1:1552:A:ILE:HG12	14	0.14
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	16	0.14
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	19	0.14
(1,467)	1:1625:A:MET:HE1	1:1625:A:MET:HA	9	0.14
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	3	0.14
(1,459)	1:1627:A:ILE:HG23	1:1627:A:ILE:H	4	0.14
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	19	0.14
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	4	0.14
(1,444)	1:1550:A:MET:HE1	1:1610:A:ILE:HA	16	0.14
(1,442)	1:1550:A:MET:HE3	1:1640:A:TRP:HB2	11	0.14
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG11	6	0.14
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG12	14	0.14
(1,389)	2:19:B:PHE:HE1	1:1572:A:ILE:HD11	14	0.14
(1,376)	2:54:B:ALA:HB1	2:52:B:ASP:H	11	0.14
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	8	0.14
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	16	0.14
(1,332)	2:55:B:LEU:HD12	2:56:B:LEU:H	17	0.14
(1,315)	2:32:B:ALA:H	2:31:B:PRO:HG3	4	0.14
(1,314)	2:45:B:GLU:H	2:55:B:LEU:HD21	12	0.14
(1,310)	2:43:B:VAL:H	2:45:B:GLU:HB2	4	0.14
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	16	0.14
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	3	0.14
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	8	0.14
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	19	0.14
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG12	17	0.14
(1,220)	2:4:B:PRO:HB2	2:2:B:TYR:HE1	19	0.14
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG12	13	0.14
(1,208)	1:1609:A:VAL:HG13	1:1590:A:LEU:H	9	0.14
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD22	9	0.14
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD21	20	0.14
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:1638:A:PHE:HD2	1:1610:A:ILE:HD13	19	0.14
(1,103)	1:1610:A:ILE:HD13	1:1590:A:LEU:H	17	0.14
(1,95)	1:1602:A:SER:HB3	1:1604:A:LEU:HD12	16	0.14
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	2	0.14
(1,18)	1:1645:A:ALA:HB2	1:1614:A:CYS:HB3	4	0.14
(1,13)	1:1547:A:VAL:HG23	1:1548:A:VAL:HA	7	0.14
(1,13)	1:1547:A:VAL:HG22	1:1548:A:VAL:HA	14	0.14
(1,12)	1:1625:A:MET:HE1	1:1623:A:ARG:HD2	5	0.14
(1,6)	1:1552:A:ILE:HD11	1:1610:A:ILE:HB	3	0.14
(3,8)	2:43:B:VAL:O	2:47:B:CYS:N	2	0.13
(1,3018)	2:18:B:GLN:HE21	1:1545:A:SER:HB3	18	0.13
(1,3002)	2:42:B:ILE:HD13	2:28:B:PHE:HE2	12	0.13
(1,2962)	2:18:B:GLN:HG2	2:26:B:PHE:HE2	6	0.13
(1,2962)	2:18:B:GLN:HG2	2:26:B:PHE:HE2	12	0.13
(1,2922)	2:61:B:ALA:HA	2:27:B:TYR:HD2	17	0.13
(1,2913)	2:27:B:TYR:HD1	2:27:B:TYR:HA	14	0.13
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	12	0.13
(1,2841)	2:13:B:LEU:HD21	2:47:B:CYS:H	20	0.13
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	12	0.13
(1,2830)	2:41:B:GLY:H	2:42:B:ILE:HG23	1	0.13
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	6	0.13
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	6	0.13
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	14	0.13
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	20	0.13
(1,2807)	2:22:B:GLY:H	2:20:B:VAL:HG12	3	0.13
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD11	5	0.13
(1,2781)	2:46:B:CYS:H	2:13:B:LEU:HD23	19	0.13
(1,2713)	2:51:B:CYS:H	2:55:B:LEU:HD21	5	0.13
(1,2657)	2:39:B:SER:H	2:38:B:ARG:HB3	6	0.13
(1,2656)	2:39:B:SER:H	2:38:B:ARG:HA	3	0.13
(1,2632)	2:38:B:ARG:H	2:38:B:ARG:HB3	10	0.13
(1,2623)	2:37:B:ARG:H	2:35:B:VAL:HA	6	0.13
(1,2606)	2:34:B:ARG:H	2:34:B:ARG:HB2	4	0.13
(1,2597)	2:33:B:SER:H	2:35:B:VAL:H	13	0.13
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	14	0.13
(1,2546)	2:7:B:THR:H	2:7:B:THR:HG23	14	0.13
(1,2540)	2:50:B:SER:H	2:49:B:ARG:HB2	4	0.13
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	9	0.13
(1,2439)	2:13:B:LEU:HD21	2:47:B:CYS:H	20	0.13
(1,2430)	2:63:B:PRO:HD2	2:63:B:PRO:HB3	14	0.13
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	3	0.13
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	8	0.13
(1,2398)	2:35:B:VAL:HA	2:35:B:VAL:HG13	6	0.13
(1,2384)	2:33:B:SER:HB3	2:34:B:ARG:H	20	0.13
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE2	7	0.13
(1,2295)	2:17:B:LEU:HD23	2:56:B:LEU:HA	5	0.13
(1,2277)	2:42:B:ILE:HD12	2:45:B:GLU:HB2	1	0.13
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG22	7	0.13
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG11	5	0.13
(1,2179)	1:1578:A:ASN:HD22	1:1592:A:TYR:HA	2	0.13
(1,2168)	1:1589:A:GLN:HB3	1:1589:A:GLN:HE21	8	0.13
(1,2167)	1:1524:A:GLY:H	1:1520:A:ASN:HB3	1	0.13
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	11	0.13
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	2	0.13
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	9	0.13
(1,2078)	1:1582:A:ARG:HA	1:1583:A:TYR:H	15	0.13
(1,2029)	1:1563:A:VAL:H	1:1561:A:PRO:HB3	15	0.13
(1,1964)	1:1568:A:GLY:H	1:1567:A:PHE:HE1	1	0.13
(1,1910)	1:1589:A:GLN:HE22	1:1609:A:VAL:HG12	1	0.13
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	1	0.13
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	16	0.13
(1,1884)	1:1570:A:THR:H	1:1570:A:THR:HB	9	0.13
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG22	6	0.13
(1,1862)	1:1635:A:THR:H	1:1635:A:THR:HG23	14	0.13
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	12	0.13
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	16	0.13
(1,1818)	1:1632:A:GLN:HG2	1:1632:A:GLN:HE21	11	0.13
(1,1818)	1:1632:A:GLN:HG3	1:1632:A:GLN:HE21	11	0.13
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	13	0.13
(1,1807)	1:1562:A:GLY:H	1:1560:A:PRO:HB2	7	0.13
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	4	0.13
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	20	0.13
(1,1787)	1:1517:A:GLN:H	1:1581:A:LEU:HD11	3	0.13
(1,1710)	1:1632:A:GLN:H	1:1631:A:LYS:HB2	12	0.13
(1,1651)	1:1617:A:GLU:H	1:1615:A:ARG:HA	9	0.13
(1,1651)	1:1617:A:GLU:H	1:1615:A:ARG:HA	15	0.13
(1,1620)	1:1558:A:ASN:H	1:1557:A:GLU:HG2	12	0.13
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	9	0.13
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	16	0.13
(1,1576)	1:1644:A:LEU:HD23	1:1644:A:LEU:H	14	0.13
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG22	8	0.13
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	3	0.13
(1,1507)	1:1532:A:LEU:H	1:1531:A:SER:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1471)	1:1551:A:SER:H	1:1550:A:MET:HG2	4	0.13
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	18	0.13
(1,1421)	1:1588:A:LEU:H	1:1645:A:ALA:HB1	1	0.13
(1,1395)	1:1591:A:VAL:H	1:1590:A:LEU:HB3	16	0.13
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	7	0.13
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	19	0.13
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	4	0.13
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	7	0.13
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	15	0.13
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	8	0.13
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	20	0.13
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	7	0.13
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	1	0.13
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	3	0.13
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	12	0.13
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	15	0.13
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	13	0.13
(1,1180)	1:1610:A:ILE:HD11	1:1610:A:ILE:H	13	0.13
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	14	0.13
(1,1145)	1:1636:A:LEU:H	1:1636:A:LEU:HB2	13	0.13
(1,1139)	1:1577:A:ALA:HB3	1:1554:A:GLY:H	8	0.13
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG23	12	0.13
(1,1058)	1:1626:A:LEU:HD21	1:1638:A:PHE:HD1	8	0.13
(1,1048)	1:1584:A:VAL:HG12	1:1584:A:VAL:H	20	0.13
(1,1042)	1:1609:A:VAL:HG13	1:1637:A:PHE:HB3	3	0.13
(1,1010)	1:1548:A:VAL:HG12	1:1542:A:TYR:HD2	20	0.13
(1,981)	1:1625:A:MET:HG2	1:1627:A:ILE:HD13	16	0.13
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	4	0.13
(1,927)	1:1571:A:ARG:HD3	1:1571:A:ARG:HE	9	0.13
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	4	0.13
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	9	0.13
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	16	0.13
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	5	0.13
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	5	0.13
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG2	13	0.13
(1,839)	1:1620:A:PRO:HD3	1:1620:A:PRO:HG3	13	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	1	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	3	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	7	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	8	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	17	0.13
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:1623:A:ARG:HD2	1:1623:A:ARG:HE	13	0.13
(1,811)	1:1514:A:ASP:HB3	1:1515:A:ASP:H	9	0.13
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	4	0.13
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	7	0.13
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	19	0.13
(1,722)	1:1581:A:LEU:HD12	1:1518:A:VAL:HB	14	0.13
(1,722)	1:1581:A:LEU:HD12	1:1518:A:VAL:HB	16	0.13
(1,665)	1:1563:A:VAL:HG21	1:1566:A:CYS:HB3	5	0.13
(1,646)	1:1529:A:LEU:HD12	1:1612:A:PHE:HZ	20	0.13
(1,638)	1:1588:A:LEU:HD21	1:1588:A:LEU:HB2	5	0.13
(1,638)	1:1588:A:LEU:HD21	1:1588:A:LEU:HB2	10	0.13
(1,631)	1:1539:A:THR:HG22	1:1549:A:TYR:HA	7	0.13
(1,631)	1:1539:A:THR:HG22	1:1549:A:TYR:HA	16	0.13
(1,631)	1:1539:A:THR:HG23	1:1549:A:TYR:HA	17	0.13
(1,630)	1:1588:A:LEU:HD22	1:1588:A:LEU:HA	1	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	2	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	4	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	8	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	11	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	15	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	18	0.13
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	19	0.13
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	2	0.13
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	5	0.13
(1,605)	1:1518:A:VAL:HG12	1:1518:A:VAL:HB	15	0.13
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	17	0.13
(1,583)	1:1540:A:ALA:HB3	1:1638:A:PHE:HE1	9	0.13
(1,582)	1:1540:A:ALA:HB2	1:1548:A:VAL:H	15	0.13
(1,581)	1:1532:A:LEU:HD23	1:1532:A:LEU:H	5	0.13
(1,562)	1:1532:A:LEU:HD22	1:1640:A:TRP:HZ2	1	0.13
(1,542)	1:1613:A:VAL:HG13	1:1641:A:HIS:HA	2	0.13
(1,494)	1:1610:A:ILE:HG22	1:1638:A:PHE:HD2	20	0.13
(1,485)	1:1577:A:ALA:HB3	1:1564:A:GLY:HA3	2	0.13
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	9	0.13
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	8	0.13
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	9	0.13
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	11	0.13
(1,471)	1:1572:A:ILE:HG22	1:1596:A:SER:HB2	6	0.13
(1,467)	1:1625:A:MET:HE2	1:1625:A:MET:HA	14	0.13
(1,459)	1:1627:A:ILE:HG22	1:1627:A:ILE:H	5	0.13
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	10	0.13
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:1550:A:MET:HE3	1:1610:A:ILE:HG13	5	0.13
(1,443)	1:1550:A:MET:HE1	1:1550:A:MET:H	12	0.13
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	16	0.13
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	18	0.13
(1,443)	1:1550:A:MET:HE3	1:1550:A:MET:H	19	0.13
(1,428)	1:1552:A:ILE:HD11	1:1550:A:MET:HG3	19	0.13
(1,410)	1:1543:A:SER:HB2	1:1546:A:GLY:H	9	0.13
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD13	16	0.13
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	1	0.13
(1,353)	2:61:B:ALA:HB1	2:60:B:CYS:HB2	13	0.13
(1,343)	2:66:B:SER:H	2:65:B:LYS:HB3	4	0.13
(1,313)	2:45:B:GLU:H	2:43:B:VAL:HB	16	0.13
(1,304)	2:54:B:ALA:H	2:53:B:LEU:HD21	1	0.13
(1,299)	2:36:B:SER:H	2:34:B:ARG:HG3	4	0.13
(1,297)	2:37:B:ARG:H	2:33:B:SER:HB2	2	0.13
(1,295)	2:35:B:VAL:H	2:34:B:ARG:HG2	7	0.13
(1,289)	2:26:B:PHE:H	2:61:B:ALA:HB2	5	0.13
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	12	0.13
(1,255)	2:4:B:PRO:HD2	2:3:B:ARG:HG3	3	0.13
(1,231)	2:46:B:CYS:H	2:55:B:LEU:HD21	18	0.13
(1,213)	1:1549:A:TYR:H	1:1566:A:CYS:HA	7	0.13
(1,207)	1:1590:A:LEU:H	1:1590:A:LEU:HD23	15	0.13
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	13	0.13
(1,203)	1:1598:A:CYS:H	1:1596:A:SER:HA	16	0.13
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD23	2	0.13
(1,191)	1:1619:A:GLY:H	1:1617:A:GLU:HB3	9	0.13
(1,179)	1:1531:A:SER:H	1:1644:A:LEU:HD13	19	0.13
(1,97)	1:1590:A:LEU:HD22	1:1578:A:ASN:H	13	0.13
(1,62)	1:1588:A:LEU:HD11	1:1645:A:ALA:HA	5	0.13
(1,46)	1:1540:A:ALA:HB3	1:1541:A:ALA:HA	18	0.13
(1,21)	1:1645:A:ALA:HB1	1:1612:A:PHE:HA	4	0.13
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	14	0.12
(3,6)	2:16:B:THR:O	2:20:B:VAL:N	19	0.12
(1,3008)	2:56:B:LEU:HD22	2:17:B:LEU:H	1	0.12
(1,3008)	2:56:B:LEU:HD23	2:17:B:LEU:H	19	0.12
(1,2951)	2:25:B:GLY:H	2:22:B:GLY:HA3	12	0.12
(1,2919)	2:60:B:CYS:H	2:60:B:CYS:HB2	18	0.12
(1,2912)	2:62:B:THR:H	2:27:B:TYR:HE1	4	0.12
(1,2886)	2:28:B:PHE:H	2:29:B:SER:H	3	0.12
(1,2864)	2:51:B:CYS:H	2:52:B:ASP:HA	7	0.12
(1,2852)	2:23:B:ASP:H	2:22:B:GLY:H	6	0.12
(1,2852)	2:23:B:ASP:H	2:22:B:GLY:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	16	0.12
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	15	0.12
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	16	0.12
(1,2782)	2:46:B:CYS:H	2:55:B:LEU:HD21	1	0.12
(1,2772)	2:66:B:SER:H	2:65:B:LYS:HA	18	0.12
(1,2761)	2:44:B:GLU:H	2:44:B:GLU:HB2	20	0.12
(1,2760)	2:44:B:GLU:H	2:48:B:PHE:HD2	11	0.12
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	3	0.12
(1,2677)	2:5:B:SER:H	2:4:B:PRO:HG3	9	0.12
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	12	0.12
(1,2639)	2:38:B:ARG:H	2:32:B:ALA:HA	7	0.12
(1,2632)	2:38:B:ARG:H	2:38:B:ARG:HB3	7	0.12
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	6	0.12
(1,2624)	2:36:B:SER:H	2:36:B:SER:HB3	1	0.12
(1,2579)	2:24:B:ARG:H	2:24:B:ARG:HD2	9	0.12
(1,2565)	2:18:B:GLN:HE22	2:18:B:GLN:HG3	5	0.12
(1,2551)	2:11:B:GLY:H	2:14:B:VAL:HG13	4	0.12
(1,2514)	2:13:B:LEU:HD23	2:13:B:LEU:HA	16	0.12
(1,2492)	2:62:B:THR:HB	2:63:B:PRO:HG3	20	0.12
(1,2479)	2:35:B:VAL:HG21	2:34:B:ARG:HA	11	0.12
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	1	0.12
(1,2392)	2:4:B:PRO:HA	2:2:B:TYR:HE2	2	0.12
(1,2323)	2:32:B:ALA:HB2	2:33:B:SER:HB2	17	0.12
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	10	0.12
(1,2303)	2:20:B:VAL:HG22	2:19:B:PHE:HE2	15	0.12
(1,2273)	2:14:B:VAL:HG22	2:26:B:PHE:HB2	6	0.12
(1,2241)	1:1527:A:PHE:HD2	1:1519:A:THR:HA	16	0.12
(1,2238)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ3	2	0.12
(1,2226)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG22	5	0.12
(1,2176)	1:1520:A:ASN:HD21	1:1523:A:THR:HG23	20	0.12
(1,2147)	1:1591:A:VAL:HG22	1:1610:A:ILE:H	13	0.12
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	8	0.12
(1,2078)	1:1582:A:ARG:HA	1:1583:A:TYR:H	20	0.12
(1,2067)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	1	0.12
(1,2067)	1:1590:A:LEU:HD21	1:1578:A:ASN:H	8	0.12
(1,1988)	1:1520:A:ASN:H	1:1523:A:THR:H	10	0.12
(1,1987)	1:1520:A:ASN:H	1:1583:A:TYR:HD2	19	0.12
(1,1906)	1:1517:A:GLN:HE22	1:1526:A:LEU:HD22	18	0.12
(1,1899)	1:1545:A:SER:H	1:1546:A:GLY:HA2	16	0.12
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	17	0.12
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD13	9	0.12
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	4	0.12
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	8	0.12
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	13	0.12
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	2	0.12
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	6	0.12
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	12	0.12
(1,1788)	1:1517:A:GLN:H	1:1581:A:LEU:HD23	6	0.12
(1,1779)	1:1546:A:GLY:HA2	1:1547:A:VAL:H	15	0.12
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG11	16	0.12
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	4	0.12
(1,1750)	1:1605:A:SER:H	1:1605:A:SER:HB3	5	0.12
(1,1722)	1:1579:A:LYS:H	1:1580:A:ARG:HG2	9	0.12
(1,1680)	1:1607:A:LYS:H	1:1635:A:THR:HG22	8	0.12
(1,1638)	1:1645:A:ALA:HB1	1:1646:A:CYS:H	8	0.12
(1,1625)	1:1509:A:LYS:HA	1:1510:A:SER:H	2	0.12
(1,1620)	1:1558:A:ASN:H	1:1557:A:GLU:HG2	13	0.12
(1,1603)	1:1553:A:CYS:H	1:1590:A:LEU:HD22	20	0.12
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	1	0.12
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	8	0.12
(1,1583)	1:1550:A:MET:H	1:1550:A:MET:HG2	19	0.12
(1,1579)	1:1637:A:PHE:H	1:1629:A:LEU:HD12	1	0.12
(1,1576)	1:1644:A:LEU:HD23	1:1644:A:LEU:H	7	0.12
(1,1544)	1:1565:A:ALA:H	1:1574:A:VAL:HG21	13	0.12
(1,1505)	1:1623:A:ARG:H	1:1623:A:ARG:HB2	19	0.12
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	19	0.12
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	3	0.12
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	10	0.12
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	11	0.12
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	17	0.12
(1,1421)	1:1588:A:LEU:H	1:1645:A:ALA:HB1	11	0.12
(1,1410)	1:1540:A:ALA:H	1:1539:A:THR:HB	15	0.12
(1,1382)	1:1647:A:GLU:H	1:1614:A:CYS:HB2	16	0.12
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	6	0.12
(1,1381)	1:1647:A:GLU:H	1:1646:A:CYS:HB3	17	0.12
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	6	0.12
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	3	0.12
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	5	0.12
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	12	0.12
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	13	0.12
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	3	0.12
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	4	0.12
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	15	0.12
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	17	0.12
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	19	0.12
(1,1264)	1:1556:A:ASN:HA	1:1557:A:GLU:H	7	0.12
(1,1263)	1:1527:A:PHE:H	1:1519:A:THR:HG21	19	0.12
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	1	0.12
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	16	0.12
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	18	0.12
(1,1250)	1:1529:A:LEU:HD11	1:1529:A:LEU:H	7	0.12
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	16	0.12
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	2	0.12
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	5	0.12
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	7	0.12
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	10	0.12
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	14	0.12
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	8	0.12
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	10	0.12
(1,1199)	1:1584:A:VAL:H	1:1583:A:TYR:HB3	15	0.12
(1,1180)	1:1610:A:ILE:HD11	1:1610:A:ILE:H	10	0.12
(1,1165)	1:1610:A:ILE:H	1:1591:A:VAL:HA	16	0.12
(1,1139)	1:1577:A:ALA:HB2	1:1554:A:GLY:H	20	0.12
(1,1137)	1:1590:A:LEU:HD11	1:1554:A:GLY:H	18	0.12
(1,1108)	1:1583:A:TYR:HD2	1:1585:A:ASP:HA	15	0.12
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	6	0.12
(1,1083)	1:1526:A:LEU:HD11	1:1517:A:GLN:HE22	19	0.12
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD22	17	0.12
(1,1064)	1:1529:A:LEU:HD12	1:1588:A:LEU:HB3	16	0.12
(1,1061)	1:1563:A:VAL:HG12	1:1566:A:CYS:HB3	20	0.12
(1,1031)	1:1577:A:ALA:HB1	1:1562:A:GLY:HA3	10	0.12
(1,996)	1:1610:A:ILE:HD12	1:1550:A:MET:HG2	2	0.12
(1,983)	1:1580:A:ARG:HD2	1:1580:A:ARG:HA	12	0.12
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	5	0.12
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	10	0.12
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	16	0.12
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	19	0.12
(1,939)	1:1539:A:THR:HA	1:1549:A:TYR:HA	12	0.12
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	18	0.12
(1,923)	1:1520:A:ASN:HB2	1:1527:A:PHE:HE2	20	0.12
(1,921)	1:1586:A:GLN:HA	1:1586:A:GLN:HB2	3	0.12
(1,921)	1:1586:A:GLN:HA	1:1586:A:GLN:HB2	14	0.12
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	10	0.12
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:1639:A:SER:HA	1:1611:A:SER:HB3	19	0.12
(1,858)	1:1647:A:GLU:HA	1:1648:A:PRO:HD3	14	0.12
(1,847)	1:1620:A:PRO:HD3	1:1619:A:GLY:HA2	3	0.12
(1,840)	1:1648:A:PRO:HD3	1:1647:A:GLU:HG2	9	0.12
(1,834)	1:1590:A:LEU:HB2	1:1590:A:LEU:HA	5	0.12
(1,834)	1:1590:A:LEU:HB2	1:1590:A:LEU:HA	10	0.12
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	5	0.12
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	13	0.12
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	11	0.12
(1,776)	1:1569:A:GLN:HG3	1:1570:A:THR:HG22	4	0.12
(1,774)	1:1509:A:LYS:HB2	1:1508:A:MET:HA	9	0.12
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	4	0.12
(1,751)	1:1635:A:THR:HG23	1:1607:A:LYS:HD3	1	0.12
(1,691)	1:1644:A:LEU:HD22	1:1527:A:PHE:HE1	14	0.12
(1,676)	1:1529:A:LEU:HD13	1:1529:A:LEU:HB3	9	0.12
(1,638)	1:1588:A:LEU:HD22	1:1588:A:LEU:HB2	7	0.12
(1,638)	1:1588:A:LEU:HD23	1:1588:A:LEU:HB2	8	0.12
(1,638)	1:1588:A:LEU:HD23	1:1588:A:LEU:HB2	15	0.12
(1,631)	1:1539:A:THR:HG21	1:1549:A:TYR:HA	3	0.12
(1,631)	1:1539:A:THR:HG23	1:1549:A:TYR:HA	4	0.12
(1,631)	1:1539:A:THR:HG23	1:1549:A:TYR:HA	9	0.12
(1,630)	1:1588:A:LEU:HD22	1:1588:A:LEU:HA	3	0.12
(1,630)	1:1588:A:LEU:HD23	1:1588:A:LEU:HA	9	0.12
(1,630)	1:1588:A:LEU:HD21	1:1588:A:LEU:HA	13	0.12
(1,630)	1:1588:A:LEU:HD22	1:1588:A:LEU:HA	17	0.12
(1,609)	1:1635:A:THR:HG21	1:1607:A:LYS:HE3	12	0.12
(1,581)	1:1532:A:LEU:HD21	1:1532:A:LEU:H	1	0.12
(1,549)	1:1574:A:VAL:HG23	1:1636:A:LEU:HB2	12	0.12
(1,512)	1:1645:A:ALA:HB2	1:1614:A:CYS:H	1	0.12
(1,512)	1:1645:A:ALA:HB2	1:1614:A:CYS:H	15	0.12
(1,509)	1:1618:A:ALA:HB3	1:1622:A:ASN:HD21	5	0.12
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	20	0.12
(1,467)	1:1625:A:MET:HE1	1:1625:A:MET:HA	8	0.12
(1,459)	1:1627:A:ILE:HG21	1:1627:A:ILE:H	8	0.12
(1,459)	1:1627:A:ILE:HG23	1:1627:A:ILE:H	16	0.12
(1,459)	1:1627:A:ILE:HG22	1:1627:A:ILE:H	17	0.12
(1,459)	1:1627:A:ILE:HG23	1:1627:A:ILE:H	18	0.12
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG13	9	0.12
(1,404)	1:1545:A:SER:H	1:1546:A:GLY:HA2	16	0.12
(1,378)	1:1632:A:GLN:HE22	2:54:B:ALA:HB1	15	0.12
(1,376)	2:54:B:ALA:HB3	2:52:B:ASP:H	17	0.12
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	19	0.12
(1,359)	2:56:B:LEU:H	2:53:B:LEU:H	16	0.12
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	17	0.12
(1,330)	2:18:B:GLN:H	2:14:B:VAL:HG23	5	0.12
(1,317)	2:53:B:LEU:H	1:1601:A:LYS:HB2	6	0.12
(1,293)	2:54:B:ALA:H	2:56:B:LEU:HD23	16	0.12
(1,267)	2:35:B:VAL:HG22	2:34:B:ARG:HD2	14	0.12
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	15	0.12
(1,260)	2:39:B:SER:H	2:38:B:ARG:HB3	16	0.12
(1,232)	2:55:B:LEU:HD23	2:46:B:CYS:HB3	14	0.12
(1,220)	2:6:B:GLU:HB3	2:2:B:TYR:HE1	16	0.12
(1,211)	1:1575:A:GLY:H	1:1576:A:LYS:HB3	14	0.12
(1,199)	1:1555:A:GLU:H	1:1562:A:GLY:HA2	6	0.12
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	4	0.12
(1,185)	1:1632:A:GLN:H	2:53:B:LEU:HD21	1	0.12
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	14	0.12
(1,147)	1:1638:A:PHE:HD2	1:1610:A:ILE:HD13	3	0.12
(1,147)	1:1638:A:PHE:HD1	1:1610:A:ILE:HD13	11	0.12
(1,125)	1:1591:A:VAL:HG21	1:1582:A:ARG:HD2	16	0.12
(1,116)	1:1613:A:VAL:HG13	1:1642:A:THR:H	9	0.12
(1,88)	1:1511:A:ASN:HB3	1:1512:A:GLU:H	8	0.12
(1,84)	1:1589:A:GLN:HG2	1:1582:A:ARG:HD3	19	0.12
(1,59)	1:1590:A:LEU:HD22	1:1578:A:ASN:HB2	13	0.12
(1,49)	1:1540:A:ALA:HB2	1:1625:A:MET:HG2	9	0.12
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB3	9	0.12
(1,24)	1:1587:A:VAL:HG23	1:1586:A:GLN:HA	17	0.12
(1,24)	1:1587:A:VAL:HG22	1:1586:A:GLN:HA	18	0.12
(1,13)	1:1547:A:VAL:HG23	1:1548:A:VAL:HA	10	0.12
(1,11)	1:1625:A:MET:HE2	1:1624:A:PRO:HA	9	0.12
(1,6)	1:1552:A:ILE:HD11	1:1610:A:ILE:HB	4	0.12
(1,3008)	2:56:B:LEU:HD21	2:17:B:LEU:H	16	0.11
(1,2992)	2:42:B:ILE:HD11	2:59:B:TYR:HE2	8	0.11
(1,2886)	2:28:B:PHE:H	2:29:B:SER:H	18	0.11
(1,2881)	2:27:B:TYR:H	2:27:B:TYR:HD1	6	0.11
(1,2864)	2:51:B:CYS:H	2:52:B:ASP:HA	20	0.11
(1,2852)	2:23:B:ASP:H	2:22:B:GLY:H	11	0.11
(1,2839)	2:33:B:SER:H	2:34:B:ARG:HB2	18	0.11
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	13	0.11
(1,2827)	2:15:B:ASP:H	2:16:B:THR:H	20	0.11
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	4	0.11
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	16	0.11
(1,2779)	2:60:B:CYS:H	2:56:B:LEU:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2745)	2:19:B:PHE:H	2:19:B:PHE:HB3	19	0.11
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD1	10	0.11
(1,2730)	2:29:B:SER:H	2:27:B:TYR:HD1	14	0.11
(1,2729)	2:29:B:SER:H	2:28:B:PHE:HD1	8	0.11
(1,2721)	2:8:B:LEU:H	2:8:B:LEU:HD21	2	0.11
(1,2705)	2:49:B:ARG:H	2:49:B:ARG:HD2	11	0.11
(1,2665)	2:28:B:PHE:H	2:27:B:TYR:HA	1	0.11
(1,2658)	2:64:B:ALA:H	2:64:B:ALA:HB2	20	0.11
(1,2648)	2:40:B:ARG:H	2:40:B:ARG:HB3	5	0.11
(1,2639)	2:38:B:ARG:H	2:32:B:ALA:HA	6	0.11
(1,2632)	2:38:B:ARG:H	2:38:B:ARG:HB3	3	0.11
(1,2632)	2:38:B:ARG:H	2:38:B:ARG:HB3	14	0.11
(1,2628)	2:36:B:SER:H	2:36:B:SER:HB2	1	0.11
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD3	1	0.11
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	2	0.11
(1,2533)	2:44:B:GLU:HB3	2:43:B:VAL:HG22	4	0.11
(1,2531)	2:61:B:ALA:HB3	2:62:B:THR:HA	1	0.11
(1,2524)	2:64:B:ALA:HA	2:65:B:LYS:HB2	4	0.11
(1,2421)	2:4:B:PRO:HD2	2:3:B:ARG:HB3	10	0.11
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	2	0.11
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	11	0.11
(1,2420)	2:63:B:PRO:HD2	2:63:B:PRO:HG3	14	0.11
(1,2397)	2:31:B:PRO:HA	2:32:B:ALA:HB1	17	0.11
(1,2391)	2:6:B:GLU:H	2:5:B:SER:HB2	12	0.11
(1,2391)	2:6:B:GLU:H	2:5:B:SER:HB2	15	0.11
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	6	0.11
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	14	0.11
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	20	0.11
(1,2324)	2:64:B:ALA:HB2	2:63:B:PRO:HA	17	0.11
(1,2318)	2:33:B:SER:H	2:32:B:ALA:HA	7	0.11
(1,2317)	2:61:B:ALA:HA	2:27:B:TYR:HE1	20	0.11
(1,2309)	2:64:B:ALA:H	2:63:B:PRO:HB3	5	0.11
(1,2308)	2:35:B:VAL:HB	2:35:B:VAL:HA	10	0.11
(1,2239)	1:1538:A:PHE:HZ	1:1640:A:TRP:HZ2	15	0.11
(1,2225)	1:1546:A:GLY:HA3	1:1547:A:VAL:HG12	14	0.11
(1,2215)	1:1644:A:LEU:HD13	1:1528:A:ASP:H	17	0.11
(1,2164)	1:1546:A:GLY:H	1:1547:A:VAL:HG13	13	0.11
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD1	1	0.11
(1,2147)	1:1591:A:VAL:HG23	1:1610:A:ILE:H	4	0.11
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	14	0.11
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	15	0.11
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2078)	1:1582:A:ARG:HA	1:1583:A:TYR:H	19	0.11
(1,2030)	1:1563:A:VAL:H	1:1555:A:GLU:HG2	9	0.11
(1,2011)	1:1555:A:GLU:H	1:1555:A:GLU:HG2	2	0.11
(1,1988)	1:1520:A:ASN:H	1:1523:A:THR:H	9	0.11
(1,1988)	1:1520:A:ASN:H	1:1523:A:THR:H	14	0.11
(1,1988)	1:1520:A:ASN:H	1:1523:A:THR:H	15	0.11
(1,1944)	1:1633:A:THR:HG21	1:1633:A:THR:H	6	0.11
(1,1944)	1:1633:A:THR:HG22	1:1633:A:THR:H	8	0.11
(1,1944)	1:1633:A:THR:HG23	1:1633:A:THR:H	13	0.11
(1,1915)	1:1618:A:ALA:HB3	1:1619:A:GLY:H	19	0.11
(1,1912)	1:1589:A:GLN:HE22	1:1591:A:VAL:HG21	12	0.11
(1,1898)	1:1545:A:SER:H	1:1545:A:SER:HB3	7	0.11
(1,1893)	1:1603:A:GLY:H	1:1604:A:LEU:HD12	16	0.11
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	15	0.11
(1,1839)	1:1602:A:SER:H	1:1603:A:GLY:H	3	0.11
(1,1818)	1:1632:A:GLN:HG2	1:1632:A:GLN:HE21	14	0.11
(1,1818)	1:1632:A:GLN:HG3	1:1632:A:GLN:HE21	14	0.11
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	3	0.11
(1,1813)	1:1569:A:GLN:HE21	1:1569:A:GLN:HA	17	0.11
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	1	0.11
(1,1799)	1:1546:A:GLY:HA2	1:1546:A:GLY:H	3	0.11
(1,1753)	1:1604:A:LEU:HD21	1:1605:A:SER:H	10	0.11
(1,1736)	1:1594:A:ASP:H	1:1605:A:SER:HB2	19	0.11
(1,1730)	1:1596:A:SER:H	1:1595:A:GLY:HA3	16	0.11
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	4	0.11
(1,1576)	1:1644:A:LEU:HD23	1:1644:A:LEU:H	13	0.11
(1,1550)	1:1606:A:TYR:H	1:1605:A:SER:HB2	13	0.11
(1,1474)	1:1551:A:SER:H	1:1565:A:ALA:HB1	17	0.11
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	15	0.11
(1,1451)	1:1547:A:VAL:HG12	1:1548:A:VAL:H	7	0.11
(1,1451)	1:1547:A:VAL:HG13	1:1548:A:VAL:H	9	0.11
(1,1405)	1:1539:A:THR:HG22	1:1540:A:ALA:H	2	0.11
(1,1405)	1:1539:A:THR:HG23	1:1540:A:ALA:H	5	0.11
(1,1323)	1:1563:A:VAL:HG23	1:1577:A:ALA:H	5	0.11
(1,1313)	1:1614:A:CYS:H	1:1613:A:VAL:HG22	13	0.11
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	8	0.11
(1,1287)	1:1635:A:THR:HG21	1:1609:A:VAL:H	1	0.11
(1,1270)	1:1557:A:GLU:H	1:1557:A:GLU:HB2	7	0.11
(1,1269)	1:1557:A:GLU:HG2	1:1557:A:GLU:H	3	0.11
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	3	0.11
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	13	0.11
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	1:1527:A:PHE:H	1:1527:A:PHE:HD2	18	0.11
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	4	0.11
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	8	0.11
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	11	0.11
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	17	0.11
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG22	2	0.11
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	20	0.11
(1,1180)	1:1610:A:ILE:HD12	1:1610:A:ILE:H	11	0.11
(1,1165)	1:1610:A:ILE:H	1:1591:A:VAL:HA	7	0.11
(1,1163)	1:1591:A:VAL:HA	1:1592:A:TYR:H	8	0.11
(1,1159)	1:1592:A:TYR:H	1:1593:A:LYS:H	3	0.11
(1,1151)	1:1615:A:ARG:H	1:1645:A:ALA:HB3	20	0.11
(1,1150)	1:1615:A:ARG:H	1:1615:A:ARG:HG3	5	0.11
(1,1137)	1:1590:A:LEU:HD12	1:1554:A:GLY:H	9	0.11
(1,1114)	1:1583:A:TYR:HE2	1:1585:A:ASP:HA	11	0.11
(1,1093)	1:1602:A:SER:H	1:1604:A:LEU:HD21	7	0.11
(1,1085)	1:1636:A:LEU:HD12	1:1574:A:VAL:HG21	2	0.11
(1,1072)	1:1590:A:LEU:HD22	1:1553:A:CYS:HA	2	0.11
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	2	0.11
(1,1057)	1:1626:A:LEU:HD21	1:1628:A:SER:H	9	0.11
(1,1029)	1:1610:A:ILE:HG22	1:1640:A:TRP:HZ3	11	0.11
(1,1003)	1:1644:A:LEU:HD23	1:1532:A:LEU:H	3	0.11
(1,1002)	1:1550:A:MET:HE2	1:1608:A:SER:HB3	7	0.11
(1,991)	1:1618:A:ALA:HB1	1:1617:A:GLU:HA	6	0.11
(1,990)	1:1636:A:LEU:HD12	1:1636:A:LEU:HB3	3	0.11
(1,990)	1:1636:A:LEU:HD12	1:1636:A:LEU:HB3	6	0.11
(1,977)	1:1508:A:MET:HE3	1:1508:A:MET:HA	2	0.11
(1,972)	1:1561:A:PRO:HA	1:1560:A:PRO:HB2	2	0.11
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	3	0.11
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	7	0.11
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	14	0.11
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	18	0.11
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	2	0.11
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	12	0.11
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	19	0.11
(1,921)	1:1586:A:GLN:HA	1:1586:A:GLN:HB2	1	0.11
(1,888)	1:1544:A:LYS:HB2	1:1544:A:LYS:HA	17	0.11
(1,841)	1:1648:A:PRO:HD2	1:1647:A:GLU:HB2	2	0.11
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	4	0.11
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	10	0.11
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	11	0.11
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	14	0.11
(1,805)	1:1585:A:ASP:HB3	1:1584:A:VAL:HG21	8	0.11
(1,776)	1:1569:A:GLN:HG2	1:1570:A:THR:HG21	2	0.11
(1,760)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD2	9	0.11
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	2	0.11
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	7	0.11
(1,759)	1:1648:A:PRO:HB2	1:1648:A:PRO:HD3	18	0.11
(1,751)	1:1635:A:THR:HG21	1:1607:A:LYS:HD3	15	0.11
(1,750)	1:1617:A:GLU:HB2	1:1618:A:ALA:H	2	0.11
(1,750)	1:1617:A:GLU:HB2	1:1618:A:ALA:H	7	0.11
(1,722)	1:1581:A:LEU:HD13	1:1518:A:VAL:HB	17	0.11
(1,720)	1:1627:A:ILE:HG12	1:1626:A:LEU:HD12	4	0.11
(1,664)	1:1607:A:LYS:HG3	1:1607:A:LYS:HE3	14	0.11
(1,650)	1:1590:A:LEU:HD21	1:1581:A:LEU:H	10	0.11
(1,644)	1:1526:A:LEU:HD12	1:1526:A:LEU:H	5	0.11
(1,631)	1:1539:A:THR:HG23	1:1549:A:TYR:HA	5	0.11
(1,630)	1:1588:A:LEU:HD22	1:1588:A:LEU:HA	10	0.11
(1,630)	1:1588:A:LEU:HD23	1:1588:A:LEU:HA	16	0.11
(1,605)	1:1518:A:VAL:HG13	1:1518:A:VAL:HB	1	0.11
(1,599)	1:1587:A:VAL:HG13	1:1611:A:SER:HB2	2	0.11
(1,589)	1:1635:A:THR:HG23	1:1637:A:PHE:HA	2	0.11
(1,581)	1:1532:A:LEU:HD23	1:1532:A:LEU:H	15	0.11
(1,562)	1:1532:A:LEU:HD23	1:1640:A:TRP:HZ2	19	0.11
(1,542)	1:1613:A:VAL:HG12	1:1641:A:HIS:HA	14	0.11
(1,504)	1:1618:A:ALA:HB1	1:1619:A:GLY:HA2	18	0.11
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	5	0.11
(1,478)	1:1552:A:ILE:HG21	1:1552:A:ILE:HG12	6	0.11
(1,478)	1:1552:A:ILE:HG23	1:1552:A:ILE:HG12	15	0.11
(1,459)	1:1627:A:ILE:HG22	1:1627:A:ILE:H	6	0.11
(1,459)	1:1627:A:ILE:HG22	1:1627:A:ILE:H	7	0.11
(1,459)	1:1627:A:ILE:HG23	1:1627:A:ILE:H	13	0.11
(1,443)	1:1550:A:MET:HE2	1:1550:A:MET:H	1	0.11
(1,420)	1:1627:A:ILE:HD13	1:1639:A:SER:HB2	6	0.11
(1,411)	1:1602:A:SER:H	1:1600:A:SER:HA	7	0.11
(1,383)	2:12:B:GLU:HG3	1:1572:A:ILE:HD11	17	0.11
(1,382)	2:12:B:GLU:HG2	1:1572:A:ILE:HD12	10	0.11
(1,368)	1:1542:A:TYR:HE1	2:19:B:PHE:HA	2	0.11
(1,366)	2:28:B:PHE:HE1	2:28:B:PHE:HA	16	0.11
(1,354)	1:1606:A:TYR:HD1	2:19:B:PHE:HZ	14	0.11
(1,301)	2:38:B:ARG:H	2:39:B:SER:HB2	2	0.11
(1,300)	2:16:B:THR:H	2:13:B:LEU:HB3	18	0.11
(1,296)	2:35:B:VAL:H	2:34:B:ARG:HD3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	2:4:B:PRO:HB3	2:3:B:ARG:HA	17	0.11
(1,276)	2:56:B:LEU:HB3	2:59:B:TYR:H	20	0.11
(1,246)	2:36:B:SER:H	2:33:B:SER:HB2	18	0.11
(1,245)	2:42:B:ILE:HD12	2:43:B:VAL:HA	12	0.11
(1,244)	2:37:B:ARG:H	2:37:B:ARG:HD3	20	0.11
(1,240)	2:22:B:GLY:H	2:20:B:VAL:HG13	1	0.11
(1,195)	1:1633:A:THR:H	1:1604:A:LEU:HD22	7	0.11
(1,190)	1:1626:A:LEU:HB3	1:1628:A:SER:H	6	0.11
(1,167)	1:1544:A:LYS:HD2	1:1544:A:LYS:H	20	0.11
(1,161)	1:1647:A:GLU:H	1:1648:A:PRO:HA	13	0.11
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	19	0.11
(1,142)	1:1581:A:LEU:HD12	1:1582:A:ARG:HG3	12	0.11
(1,32)	1:1547:A:VAL:HG21	1:1549:A:TYR:HB3	11	0.11
(1,32)	1:1547:A:VAL:HG22	1:1549:A:TYR:HB3	16	0.11
(1,28)	1:1609:A:VAL:HG23	1:1607:A:LYS:HB3	19	0.11
(1,22)	1:1584:A:VAL:HG13	1:1583:A:TYR:H	18	0.11
(1,17)	1:1577:A:ALA:HB3	1:1553:A:CYS:H	10	0.11
(1,6)	1:1552:A:ILE:HD13	1:1610:A:ILE:HB	7	0.11
(1,2810)	2:9:B:CYS:H	2:8:B:LEU:HA	1	0.1
(1,2793)	2:58:B:THR:H	2:55:B:LEU:HD12	17	0.1
(1,2733)	2:29:B:SER:H	2:27:B:TYR:HB3	8	0.1
(1,2715)	2:52:B:ASP:H	2:55:B:LEU:H	6	0.1
(1,2689)	2:6:B:GLU:H	2:7:B:THR:HG21	9	0.1
(1,2604)	2:34:B:ARG:H	2:33:B:SER:HB2	19	0.1
(1,2597)	2:33:B:SER:H	2:35:B:VAL:H	17	0.1
(1,2588)	2:62:B:THR:H	2:24:B:ARG:HD2	16	0.1
(1,2564)	2:18:B:GLN:HE22	2:18:B:GLN:HG2	16	0.1
(1,2534)	2:44:B:GLU:HB2	2:43:B:VAL:HG21	17	0.1
(1,2494)	2:37:B:ARG:HG2	2:37:B:ARG:HA	18	0.1
(1,2490)	2:63:B:PRO:HD3	2:62:B:THR:HB	18	0.1
(1,2480)	2:13:B:LEU:HD11	2:13:B:LEU:HA	4	0.1
(1,2479)	2:35:B:VAL:HG23	2:34:B:ARG:HA	17	0.1
(1,2454)	2:35:B:VAL:HG21	2:34:B:ARG:HA	5	0.1
(1,2388)	2:33:B:SER:HB2	2:35:B:VAL:HG21	3	0.1
(1,2385)	2:66:B:SER:HB3	2:66:B:SER:H	19	0.1
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	9	0.1
(1,2342)	2:18:B:GLN:HB3	2:21:B:CYS:H	20	0.1
(1,2323)	2:32:B:ALA:HB2	2:33:B:SER:HB2	15	0.1
(1,2318)	2:33:B:SER:H	2:32:B:ALA:HA	9	0.1
(1,2310)	2:20:B:VAL:HG11	2:21:B:CYS:HB3	11	0.1
(1,2309)	2:64:B:ALA:H	2:63:B:PRO:HB3	4	0.1
(1,2277)	2:42:B:ILE:HD13	2:45:B:GLU:HB2	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2269)	2:8:B:LEU:H	2:7:B:THR:HG22	6	0.1
(1,2236)	1:1549:A:TYR:HD1	1:1556:A:ASN:HD21	2	0.1
(1,2236)	1:1549:A:TYR:HD1	1:1556:A:ASN:HD21	5	0.1
(1,2236)	1:1549:A:TYR:HD1	1:1556:A:ASN:HD21	15	0.1
(1,2186)	1:1556:A:ASN:HD22	1:1537:A:GLY:HA2	19	0.1
(1,2154)	1:1638:A:PHE:H	1:1638:A:PHE:HD2	3	0.1
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	6	0.1
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	7	0.1
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	10	0.1
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	16	0.1
(1,2138)	1:1640:A:TRP:H	1:1641:A:HIS:HB3	17	0.1
(1,2079)	1:1588:A:LEU:HD12	1:1583:A:TYR:H	5	0.1
(1,2069)	1:1578:A:ASN:H	1:1564:A:GLY:HA2	18	0.1
(1,1975)	1:1538:A:PHE:H	1:1538:A:PHE:HD2	5	0.1
(1,1944)	1:1633:A:THR:HG23	1:1633:A:THR:H	5	0.1
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	1	0.1
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	11	0.1
(1,1889)	1:1603:A:GLY:H	1:1602:A:SER:HA	14	0.1
(1,1861)	1:1635:A:THR:H	1:1630:A:ASP:HB3	2	0.1
(1,1851)	1:1621:A:THR:H	1:1620:A:PRO:HD2	16	0.1
(1,1775)	1:1564:A:GLY:H	1:1563:A:VAL:HG11	17	0.1
(1,1702)	1:1571:A:ARG:H	1:1569:A:GLN:H	10	0.1
(1,1666)	1:1639:A:SER:H	1:1639:A:SER:HB2	12	0.1
(1,1651)	1:1617:A:GLU:H	1:1615:A:ARG:HA	3	0.1
(1,1651)	1:1617:A:GLU:H	1:1615:A:ARG:HA	8	0.1
(1,1638)	1:1645:A:ALA:HB3	1:1646:A:CYS:H	7	0.1
(1,1638)	1:1645:A:ALA:HB2	1:1646:A:CYS:H	19	0.1
(1,1592)	1:1518:A:VAL:H	1:1518:A:VAL:HB	9	0.1
(1,1574)	1:1518:A:VAL:HG13	1:1519:A:THR:H	1	0.1
(1,1534)	1:1572:A:ILE:HG21	1:1573:A:SER:H	18	0.1
(1,1532)	1:1573:A:SER:H	1:1573:A:SER:HB2	8	0.1
(1,1493)	1:1511:A:ASN:H	1:1510:A:SER:HA	1	0.1
(1,1462)	1:1611:A:SER:H	1:1639:A:SER:HA	2	0.1
(1,1372)	1:1572:A:ILE:H	1:1572:A:ILE:HG13	10	0.1
(1,1357)	1:1582:A:ARG:H	1:1584:A:VAL:HG23	13	0.1
(1,1337)	1:1600:A:SER:H	1:1601:A:LYS:H	13	0.1
(1,1333)	1:1569:A:GLN:H	1:1568:A:GLY:H	15	0.1
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	8	0.1
(1,1298)	1:1583:A:TYR:H	1:1582:A:ARG:HG2	10	0.1
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	1	0.1
(1,1295)	1:1583:A:TYR:H	1:1583:A:TYR:HB3	14	0.1
(1,1278)	1:1601:A:LYS:HE2	1:1601:A:LYS:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:1618:A:ALA:HA	1:1618:A:ALA:H	9	0.1
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	5	0.1
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	8	0.1
(1,1262)	1:1527:A:PHE:H	1:1526:A:LEU:HG	10	0.1
(1,1250)	1:1529:A:LEU:HD11	1:1529:A:LEU:H	16	0.1
(1,1250)	1:1529:A:LEU:HD13	1:1529:A:LEU:H	18	0.1
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	13	0.1
(1,1247)	1:1529:A:LEU:H	1:1529:A:LEU:HG	15	0.1
(1,1229)	1:1641:A:HIS:H	1:1642:A:THR:HG22	11	0.1
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG23	7	0.1
(1,1216)	1:1641:A:HIS:H	1:1613:A:VAL:HG22	17	0.1
(1,1209)	1:1630:A:ASP:H	1:1630:A:ASP:HB3	18	0.1
(1,1203)	1:1588:A:LEU:HD22	1:1584:A:VAL:H	17	0.1
(1,1159)	1:1592:A:TYR:H	1:1593:A:LYS:H	18	0.1
(1,1159)	1:1592:A:TYR:H	1:1593:A:LYS:H	19	0.1
(1,1139)	1:1577:A:ALA:HB1	1:1554:A:GLY:H	7	0.1
(1,1138)	1:1554:A:GLY:H	1:1552:A:ILE:HG22	13	0.1
(1,1136)	1:1590:A:LEU:HD23	1:1554:A:GLY:H	10	0.1
(1,1079)	1:1636:A:LEU:HD23	1:1626:A:LEU:HD13	18	0.1
(1,1057)	1:1626:A:LEU:HD23	1:1628:A:SER:H	17	0.1
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	1	0.1
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	6	0.1
(1,942)	1:1567:A:PHE:HA	1:1568:A:GLY:H	9	0.1
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	7	0.1
(1,926)	1:1526:A:LEU:HA	1:1527:A:PHE:H	15	0.1
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD2	3	0.1
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD3	3	0.1
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD2	15	0.1
(1,879)	1:1642:A:THR:HA	1:1643:A:PRO:HD3	15	0.1
(1,824)	1:1581:A:LEU:HB3	1:1581:A:LEU:H	2	0.1
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	15	0.1
(1,810)	1:1585:A:ASP:HB2	1:1585:A:ASP:H	20	0.1
(1,727)	1:1629:A:LEU:HD23	1:1631:A:LYS:HA	10	0.1
(1,706)	1:1604:A:LEU:H	1:1604:A:LEU:HD12	11	0.1
(1,697)	1:1644:A:LEU:HD13	1:1529:A:LEU:HD12	19	0.1
(1,676)	1:1529:A:LEU:HD13	1:1529:A:LEU:HB3	5	0.1
(1,644)	1:1526:A:LEU:HD13	1:1526:A:LEU:H	10	0.1
(1,638)	1:1588:A:LEU:HD23	1:1588:A:LEU:HB2	13	0.1
(1,631)	1:1539:A:THR:HG21	1:1549:A:TYR:HA	14	0.1
(1,622)	1:1644:A:LEU:HD12	1:1532:A:LEU:HD22	20	0.1
(1,596)	1:1529:A:LEU:HD22	1:1645:A:ALA:HA	18	0.1
(1,583)	1:1540:A:ALA:HB3	1:1638:A:PHE:HE1	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:1610:A:ILE:HG22	1:1590:A:LEU:HB3	13	0.1
(1,467)	1:1625:A:MET:HE1	1:1625:A:MET:HA	17	0.1
(1,435)	1:1610:A:ILE:HD12	1:1610:A:ILE:HG13	9	0.1
(1,435)	1:1610:A:ILE:HD11	1:1610:A:ILE:HG13	17	0.1
(1,414)	1:1615:A:ARG:H	1:1613:A:VAL:HG11	17	0.1
(1,385)	1:1572:A:ILE:HD11	2:12:B:GLU:HB2	1	0.1
(1,385)	1:1572:A:ILE:HD12	2:12:B:GLU:HB2	1	0.1
(1,385)	1:1572:A:ILE:HD13	2:12:B:GLU:HB2	1	0.1
(1,370)	2:18:B:GLN:HG2	1:1569:A:GLN:HE21	3	0.1
(1,310)	2:43:B:VAL:H	2:45:B:GLU:HB2	8	0.1
(1,217)	1:1640:A:TRP:H	1:1613:A:VAL:HG11	19	0.1
(1,166)	1:1589:A:GLN:H	1:1588:A:LEU:HB3	20	0.1
(1,162)	1:1548:A:VAL:HB	1:1540:A:ALA:H	3	0.1
(1,149)	1:1638:A:PHE:HD2	1:1540:A:ALA:HB3	11	0.1
(1,144)	1:1579:A:LYS:HD3	1:1578:A:ASN:HA	13	0.1
(1,19)	1:1618:A:ALA:HB1	1:1643:A:PRO:HB3	9	0.1
(1,2)	1:1552:A:ILE:HD13	1:1592:A:TYR:HD2	13	0.1

10 Dihedral-angle violation analysis

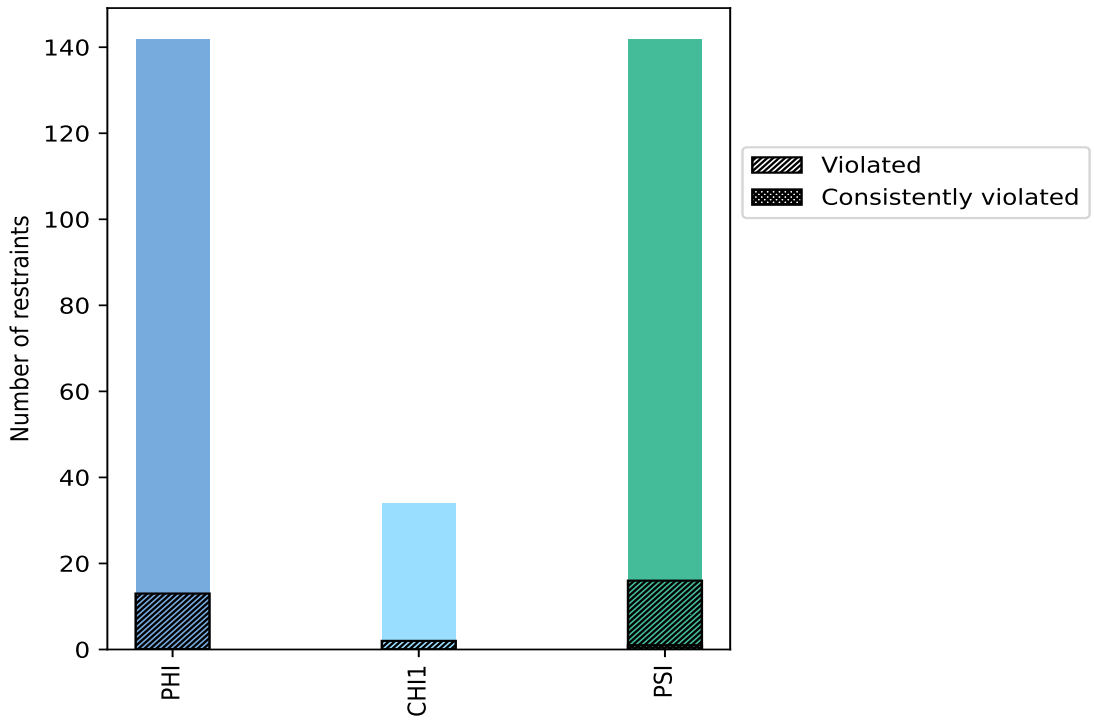
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	142	44.7	13	9.2	4.1	0	0.0	0.0
CHI1	34	10.7	2	5.9	0.6	0	0.0	0.0
PSI	142	44.7	16	11.3	5.0	1	0.7	0.3
Total	318	100.0	31	9.7	9.7	1	0.3	0.3

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



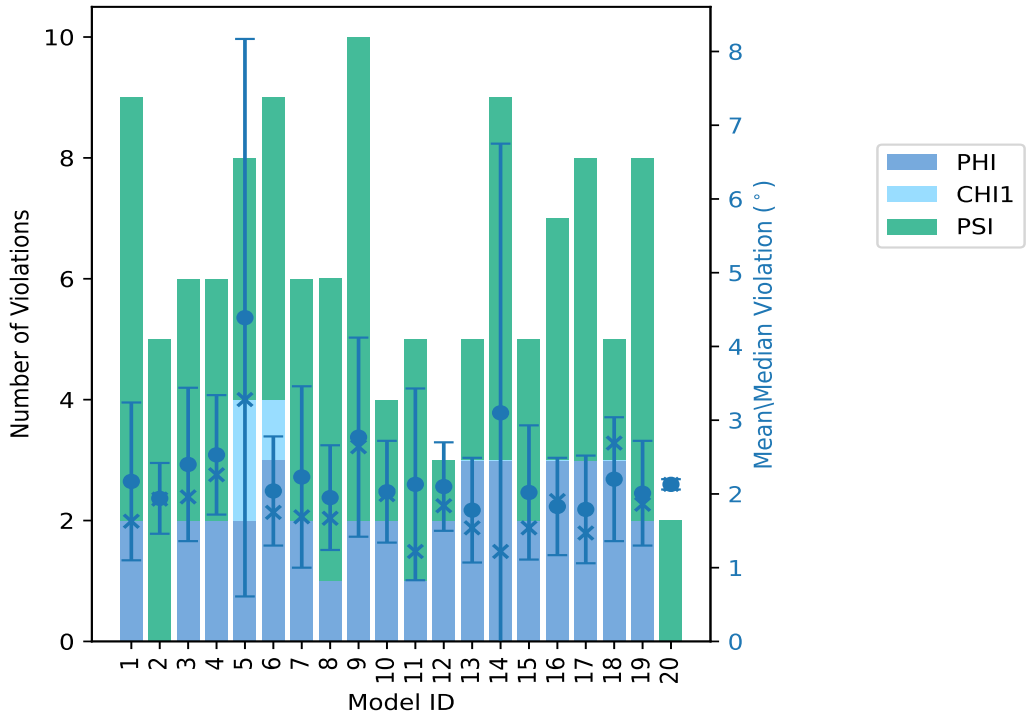
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	CHI1	PSI	Total				
1	2	0	7	9	2.17	4.68	1.07	1.63
2	0	0	5	5	1.94	2.69	0.48	1.93
3	2	0	4	6	2.4	4.17	1.04	1.96
4	2	0	4	6	2.53	3.84	0.81	2.26
5	2	2	4	8	4.39	14.02	3.78	3.28
6	3	1	5	9	2.04	3.3	0.74	1.75
7	2	0	4	6	2.23	4.5	1.23	1.69
8	1	0	5	6	1.95	3.26	0.71	1.67
9	2	0	8	10	2.77	5.72	1.35	2.64
10	2	0	2	4	2.03	2.86	0.69	1.99
11	1	0	4	5	2.13	4.21	1.3	1.22
12	2	0	1	3	2.1	2.93	0.6	1.84
13	3	0	2	5	1.78	3.16	0.71	1.54
14	3	0	6	9	3.1	12.91	3.65	1.22
15	2	0	3	5	2.02	3.49	0.91	1.54
16	3	0	4	7	1.83	2.63	0.66	1.91
17	3	0	5	8	1.79	3.28	0.73	1.47
18	3	0	2	5	2.2	3.13	0.84	2.69
19	2	0	6	8	2.01	3.56	0.71	1.86
20	0	0	2	2	2.13	2.2	0.07	2.13

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
5	1	5	11	1	5.0
1	1	1	3	2	10.0
1	0	4	5	3	15.0
3	0	2	5	4	20.0
1	0	0	1	5	25.0
1	0	0	1	6	30.0
1	0	0	1	7	35.0
0	0	0	0	8	40.0
0	0	1	1	9	45.0
0	0	1	1	10	50.0
0	0	0	0	11	55.0

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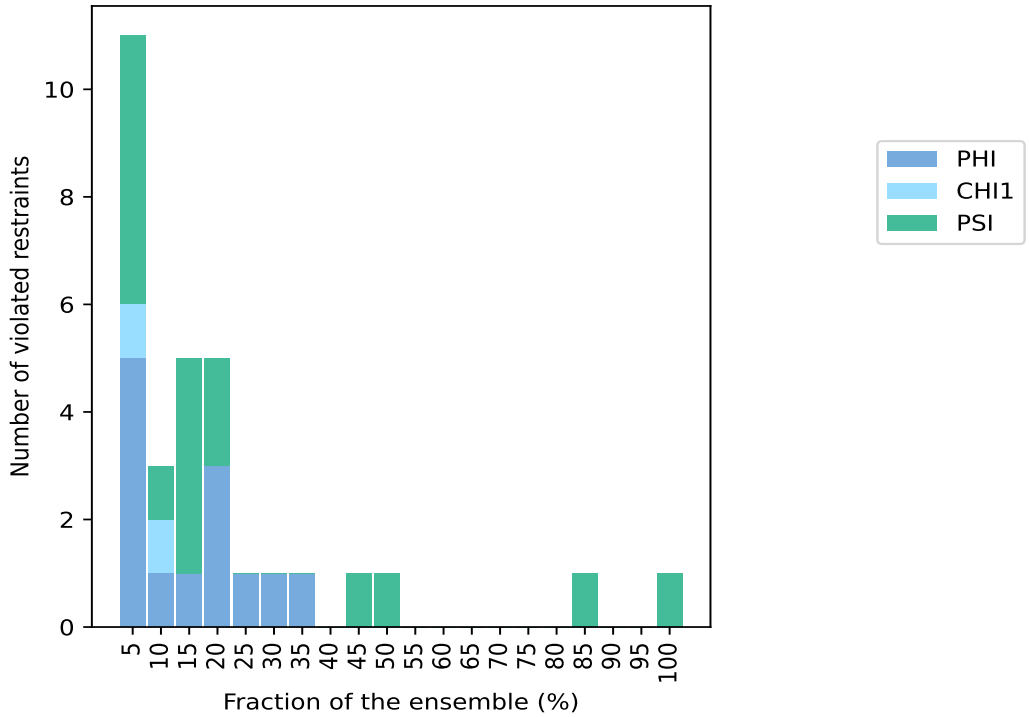
Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	0	0	16	80.0
0	0	1	1	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	1	1	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

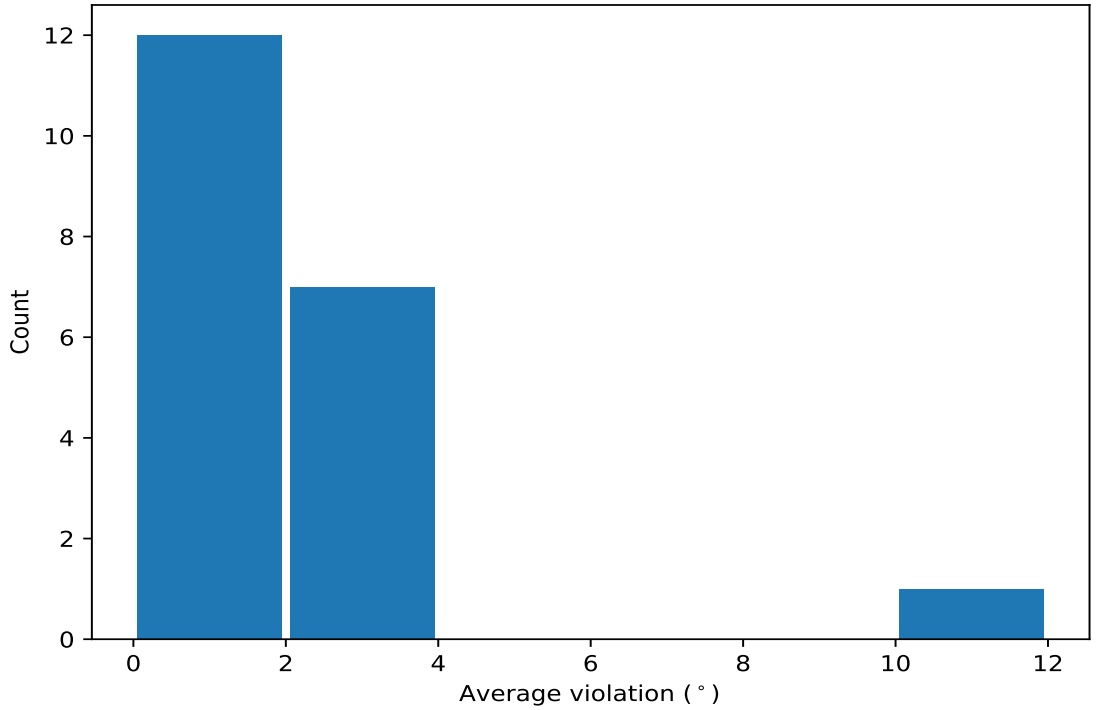


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

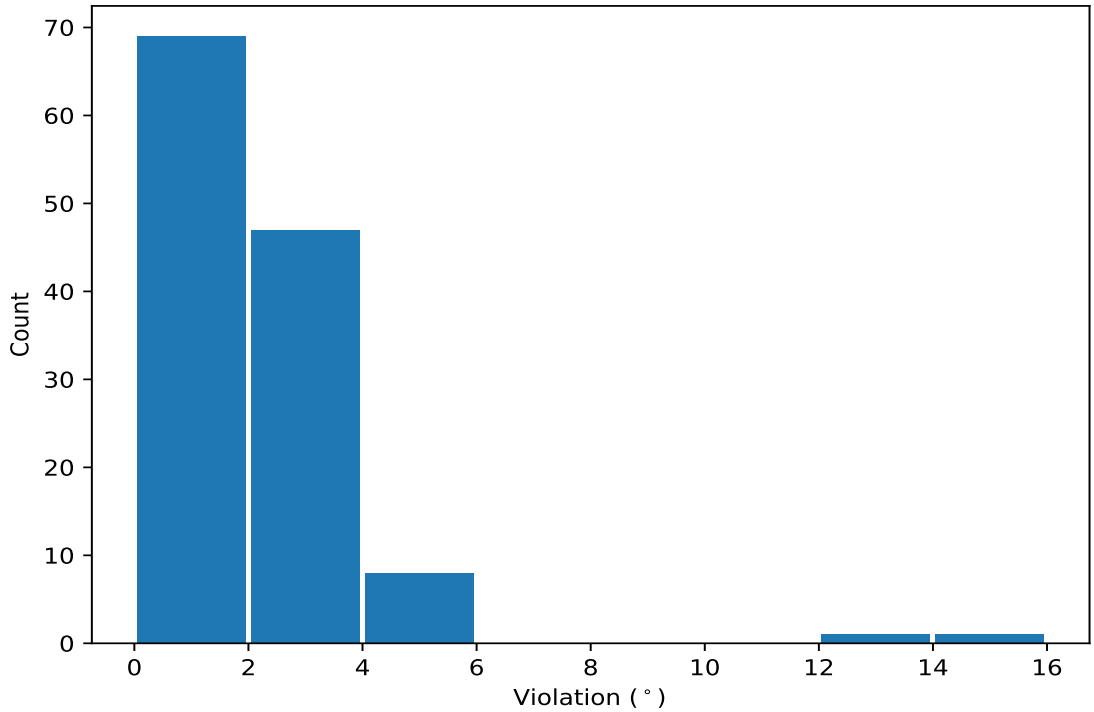
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	20	3.11	0.96	3.0
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	17	2.34	0.84	2.4
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	10	2.05	0.74	1.7
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	9	2.97	1.01	3.2
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	7	1.53	0.26	1.5
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	6	1.38	0.27	1.3
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	5	1.77	0.84	1.1
(1,45)	2:37:B:ARG:N	2:37:B:ARG:CA	2:37:B:ARG:C	2:38:B:ARG:N	4	3.11	0.33	3.0
(1,173)	1:1569:A:GLN:C	1:1570:A:THR:N	1:1570:A:THR:CA	1:1570:A:THR:C	4	2.54	0.54	2.4
(1,37)	2:30:B:ARG:N	2:30:B:ARG:CA	2:30:B:ARG:C	2:31:B:PRO:N	4	2.22	0.54	2.0
(1,185)	1:1581:A:LEU:C	1:1582:A:ARG:N	1:1582:A:ARG:CA	1:1582:A:ARG:C	4	1.89	0.67	1.7
(1,169)	1:1566:A:CYS:C	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:C	4	1.22	0.16	1.2
(1,294)	1:1647:A:GLU:N	1:1647:A:GLU:CA	1:1647:A:GLU:C	1:1648:A:PRO:N	3	10.88	3.68	12.9
(1,296)	1:1648:A:PRO:N	1:1648:A:PRO:CA	1:1648:A:PRO:C	1:1649:A:GLU:N	3	1.9	0.44	1.9
(1,93)	1:1517:A:GLN:N	1:1517:A:GLN:CA	1:1517:A:GLN:C	1:1518:A:VAL:N	3	1.49	0.26	1.6
(1,5)	2:7:B:THR:N	2:7:B:THR:CA	2:7:B:THR:C	2:8:B:LEU:N	3	1.38	0.24	1.4
(1,239)	1:1614:A:CYS:C	1:1615:A:ARG:N	1:1615:A:ARG:CA	1:1615:A:ARG:C	3	1.34	0.17	1.4
(1,83)	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:CB	2:15:B:ASP:CG	2	1.9	0.15	1.9
(1,26)	2:19:B:PHE:C	2:20:B:VAL:N	2:20:B:VAL:CA	2:20:B:VAL:C	2	1.42	0.08	1.4
(1,212)	1:1597:A:PRO:N	1:1597:A:PRO:CA	1:1597:A:PRO:C	1:1598:A:CYS:N	2	1.06	0.01	1.0

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,294)	1:1647:A:GLU:N	1:1647:A:GLU:CA	1:1647:A:GLU:C	1:1648:A:PRO:N	5	14.02
(1,294)	1:1647:A:GLU:N	1:1647:A:GLU:CA	1:1647:A:GLU:C	1:1648:A:PRO:N	14	12.91
(1,294)	1:1647:A:GLU:N	1:1647:A:GLU:CA	1:1647:A:GLU:C	1:1648:A:PRO:N	9	5.72
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	5	4.92
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	1	4.68
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	7	4.5
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	14	4.39
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	11	4.21
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	3	4.17
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	9	4.06
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	4	3.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	2:37:B:ARG:N	2:37:B:ARG:CA	2:37:B:ARG:C	2:38:B:ARG:N	9	3.57
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	19	3.56
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	5	3.53
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	15	3.49
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	14	3.42
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	3	3.4
(1,173)	1:1569:A:GLN:C	1:1570:A:THR:N	1:1570:A:THR:CA	1:1570:A:THR:C	5	3.37
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	4	3.31
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	6	3.3
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	17	3.28
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	8	3.26
(1,45)	2:37:B:ARG:N	2:37:B:ARG:CA	2:37:B:ARG:C	2:38:B:ARG:N	7	3.22
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	5	3.19
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	13	3.16
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	18	3.13
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	11	3.09
(1,37)	2:30:B:ARG:N	2:30:B:ARG:CA	2:30:B:ARG:C	2:31:B:PRO:N	6	3.09
(1,45)	2:37:B:ARG:N	2:37:B:ARG:CA	2:37:B:ARG:C	2:38:B:ARG:N	1	2.95
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	1	2.93
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	12	2.93
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	9	2.9
(1,185)	1:1581:A:LEU:C	1:1582:A:ARG:N	1:1582:A:ARG:CA	1:1582:A:ARG:C	5	2.89
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	10	2.86
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	18	2.79
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	18	2.69
(1,45)	2:37:B:ARG:N	2:37:B:ARG:CA	2:37:B:ARG:C	2:38:B:ARG:N	2	2.69
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	9	2.68
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	17	2.68
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	15	2.67
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	4	2.66
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	16	2.63
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	9	2.61
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	19	2.58
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	10	2.55
(1,173)	1:1569:A:GLN:C	1:1570:A:THR:N	1:1570:A:THR:CA	1:1570:A:THR:C	16	2.52
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	8	2.47
(1,173)	1:1569:A:GLN:C	1:1570:A:THR:N	1:1570:A:THR:CA	1:1570:A:THR:C	6	2.44
(1,296)	1:1648:A:PRO:N	1:1648:A:PRO:CA	1:1648:A:PRO:C	1:1649:A:GLU:N	9	2.43
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	16	2.42
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	20	2.2
(1,37)	2:30:B:ARG:N	2:30:B:ARG:CA	2:30:B:ARG:C	2:31:B:PRO:N	2	2.17
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	6	2.14
(1,185)	1:1581:A:LEU:C	1:1582:A:ARG:N	1:1582:A:ARG:CA	1:1582:A:ARG:C	3	2.08
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	20	2.07
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	19	2.07
(1,83)	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:CB	2:15:B:ASP:CG	5	2.05
(1,37)	2:30:B:ARG:N	2:30:B:ARG:CA	2:30:B:ARG:C	2:31:B:PRO:N	19	1.97
(1,296)	1:1648:A:PRO:N	1:1648:A:PRO:CA	1:1648:A:PRO:C	1:1649:A:GLU:N	2	1.93
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	16	1.91
(1,173)	1:1569:A:GLN:C	1:1570:A:THR:N	1:1570:A:THR:CA	1:1570:A:THR:C	4	1.85
(1,215)	1:1600:A:SER:C	1:1601:A:LYS:N	1:1601:A:LYS:CA	1:1601:A:LYS:C	12	1.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	3	1.83
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	7	1.82
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	4	1.81
(1,171)	1:1568:A:GLY:C	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	17	1.8
(1,127)	1:1535:A:ARG:N	1:1535:A:ARG:CA	1:1535:A:ARG:C	1:1536:A:ALA:N	19	1.76
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	6	1.75
(1,83)	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:CB	2:15:B:ASP:CG	6	1.74
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	6	1.73
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	4	1.72
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	8	1.7
(1,93)	1:1517:A:GLN:N	1:1517:A:GLN:CA	1:1517:A:GLN:C	1:1518:A:VAL:N	1	1.67
(1,93)	1:1517:A:GLN:N	1:1517:A:GLN:CA	1:1517:A:GLN:C	1:1518:A:VAL:N	3	1.67
(1,5)	2:7:B:THR:N	2:7:B:THR:CA	2:7:B:THR:C	2:8:B:LEU:N	8	1.65
(1,37)	2:30:B:ARG:N	2:30:B:ARG:CA	2:30:B:ARG:C	2:31:B:PRO:N	1	1.63
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	2	1.61
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	1	1.59
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	13	1.59
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	14	1.58
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	7	1.56
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	13	1.54
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	15	1.54
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	12	1.54
(1,26)	2:19:B:PHE:C	2:20:B:VAL:N	2:20:B:VAL:CA	2:20:B:VAL:C	17	1.51
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	13	1.5
(1,239)	1:1614:A:CYS:C	1:1615:A:ARG:N	1:1615:A:ARG:CA	1:1615:A:ARG:C	8	1.49
(1,169)	1:1566:A:CYS:C	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:C	1	1.46
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	9	1.43
(1,239)	1:1614:A:CYS:C	1:1615:A:ARG:N	1:1615:A:ARG:CA	1:1615:A:ARG:C	19	1.43
(1,209)	1:1595:A:GLY:C	1:1596:A:SER:N	1:1596:A:SER:CA	1:1596:A:SER:C	17	1.43
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	10	1.43
(1,5)	2:7:B:THR:N	2:7:B:THR:CA	2:7:B:THR:C	2:8:B:LEU:N	1	1.43
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	19	1.37
(1,296)	1:1648:A:PRO:N	1:1648:A:PRO:CA	1:1648:A:PRO:C	1:1649:A:GLU:N	19	1.35
(1,185)	1:1581:A:LEU:C	1:1582:A:ARG:N	1:1582:A:ARG:CA	1:1582:A:ARG:C	18	1.35
(1,26)	2:19:B:PHE:C	2:20:B:VAL:N	2:20:B:VAL:CA	2:20:B:VAL:C	15	1.34
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	17	1.33
(1,169)	1:1566:A:CYS:C	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:C	10	1.28
(1,137)	1:1542:A:TYR:N	1:1542:A:TYR:CA	1:1542:A:TYR:C	1:1543:A:SER:N	2	1.28
(1,206)	1:1592:A:TYR:N	1:1592:A:TYR:CA	1:1592:A:TYR:C	1:1593:A:LYS:N	17	1.26
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	3	1.24
(1,185)	1:1581:A:LEU:C	1:1582:A:ARG:N	1:1582:A:ARG:CA	1:1582:A:ARG:C	11	1.22
(1,142)	1:1544:A:LYS:C	1:1545:A:SER:N	1:1545:A:SER:CA	1:1545:A:SER:C	14	1.22
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	9	1.2
(1,246)	1:1623:A:ARG:N	1:1623:A:ARG:CA	1:1623:A:ARG:C	1:1624:A:PRO:N	14	1.19
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	1	1.18
(1,172)	1:1569:A:GLN:N	1:1569:A:GLN:CA	1:1569:A:GLN:C	1:1570:A:THR:N	7	1.17
(1,182)	1:1580:A:ARG:N	1:1580:A:ARG:CA	1:1580:A:ARG:C	1:1581:A:LEU:N	6	1.16
(1,305)	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:CB	1:1567:A:PHE:CG	5	1.14
(1,242)	1:1617:A:GLU:N	1:1617:A:GLU:CA	1:1617:A:GLU:C	1:1618:A:ALA:N	16	1.12
(1,93)	1:1517:A:GLN:N	1:1517:A:GLN:CA	1:1517:A:GLN:C	1:1518:A:VAL:N	8	1.12
(1,292)	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	1:1647:A:GLU:N	9	1.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,239)	1:1614:A:CYS:C	1:1615:A:ARG:N	1:1615:A:ARG:CA	1:1615:A:ARG:C	13	1.11
(1,169)	1:1566:A:CYS:C	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:C	16	1.11
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	7	1.1
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	14	1.09
(1,291)	1:1645:A:ALA:C	1:1646:A:CYS:N	1:1646:A:CYS:CA	1:1646:A:CYS:C	15	1.08
(1,144)	1:1546:A:GLY:C	1:1547:A:VAL:N	1:1547:A:VAL:CA	1:1547:A:VAL:C	16	1.08
(1,212)	1:1597:A:PRO:N	1:1597:A:PRO:CA	1:1597:A:PRO:C	1:1598:A:CYS:N	14	1.06
(1,5)	2:7:B:THR:N	2:7:B:THR:CA	2:7:B:THR:C	2:8:B:LEU:N	11	1.06
(1,212)	1:1597:A:PRO:N	1:1597:A:PRO:CA	1:1597:A:PRO:C	1:1598:A:CYS:N	11	1.05
(1,169)	1:1566:A:CYS:C	1:1567:A:PHE:N	1:1567:A:PHE:CA	1:1567:A:PHE:C	18	1.04
(1,219)	1:1602:A:SER:C	1:1603:A:GLY:N	1:1603:A:GLY:CA	1:1603:A:GLY:C	6	1.03
(1,159)	1:1558:A:ASN:C	1:1559:A:CYS:N	1:1559:A:CYS:CA	1:1559:A:CYS:C	14	1.03
(1,190)	1:1584:A:VAL:N	1:1584:A:VAL:CA	1:1584:A:VAL:C	1:1585:A:ASP:N	17	1.01