



Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 11:23 AM EDT

PDB ID : 2M41
BMRB ID : 18982
Title : Solution Structure of the AXH domain of Ataxin-1 in complex with ligand peptide from Capicua
Authors : de Chiara, C.; Kelly, G.; Pastore, A.
Deposited on : 2013-01-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

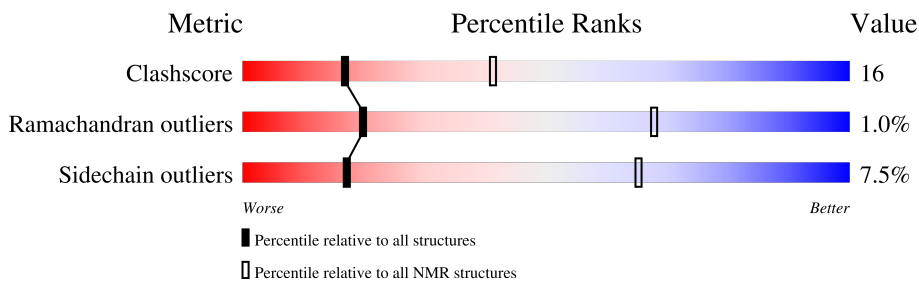
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	15	
2	B	126	

2 Ensemble composition and analysis i

This entry contains 15 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:35-A:43, B:571-B:605, B:609-B:689 (125)	0.46	14

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 8, 11, 12, 15
2	3, 6, 10, 13, 14
3	2, 5, 9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2138 atoms, of which 1065 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein capicua homolog.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	15	246	86	122	19	19	0

- Molecule 2 is a protein called Ataxin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	123	1892	605	943	152	187	5	0

There are 3 discrepancies between the modelled and reference sequences:

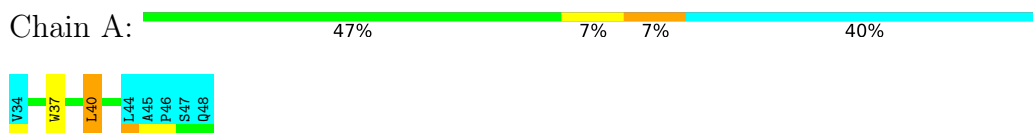
Chain	Residue	Modelled	Actual	Comment	Reference
B	564	GLY	-	expression tag	UNP P54253
B	565	ALA	-	expression tag	UNP P54253
B	566	MET	-	expression tag	UNP P54253

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: Protein capicua homolog



- Molecule 2: Ataxin-1

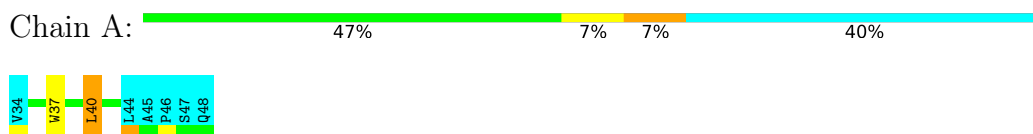


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein capicua homolog



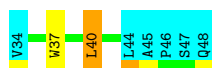
- Molecule 2: Ataxin-1



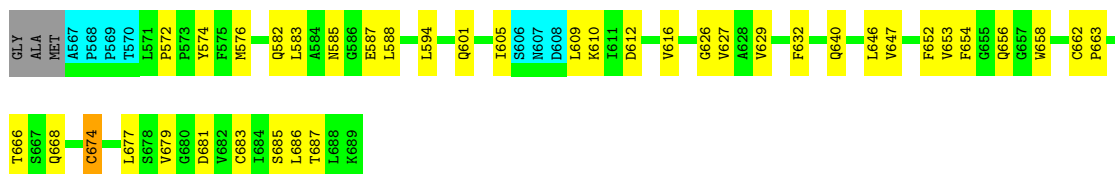


4.2.2 Score per residue for model 2

- Molecule 1: Protein capicua homolog

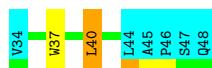


- Molecule 2: Ataxin-1

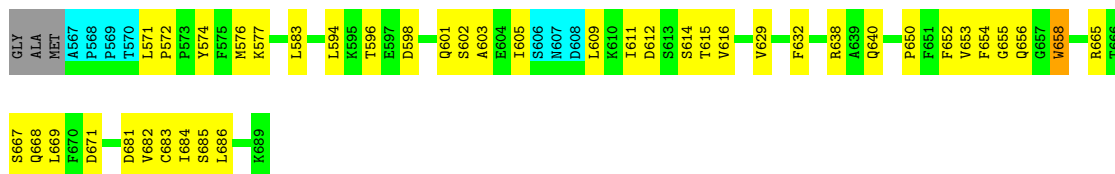


4.2.3 Score per residue for model 3

- Molecule 1: Protein capicua homolog

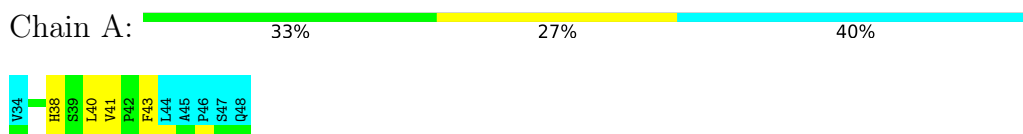


- Molecule 2: Ataxin-1

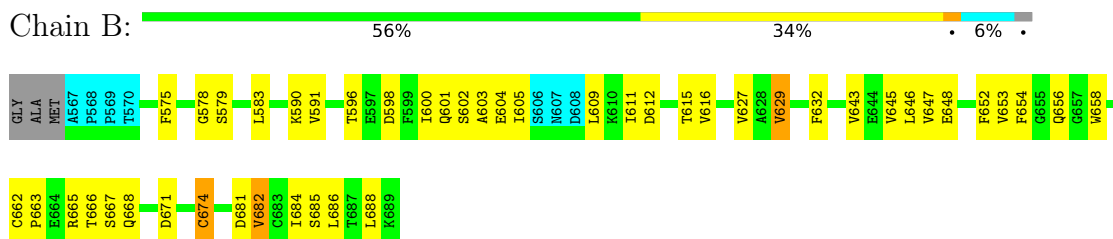


4.2.4 Score per residue for model 4

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1

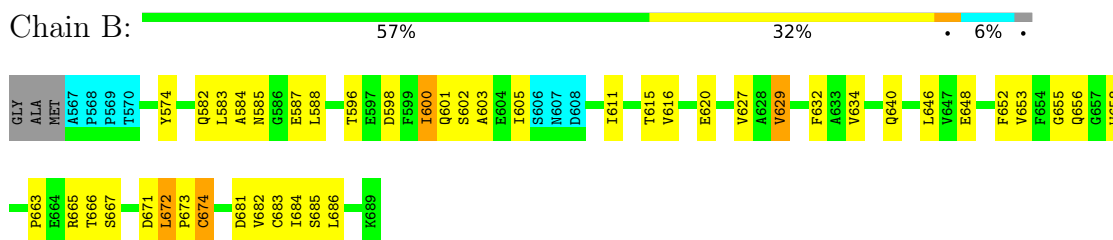


4.2.5 Score per residue for model 5

- Molecule 1: Protein capicua homolog

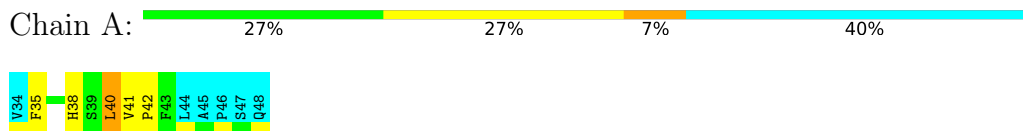


- Molecule 2: Ataxin-1

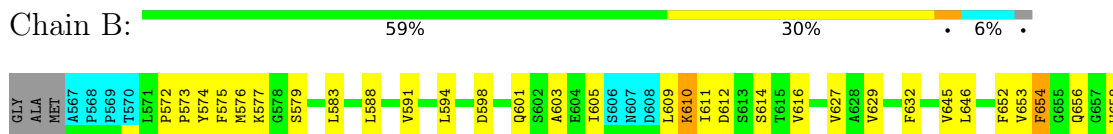


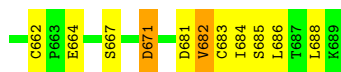
4.2.6 Score per residue for model 6

- Molecule 1: Protein capicua homolog



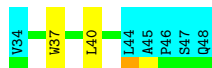
- Molecule 2: Ataxin-1



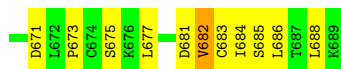
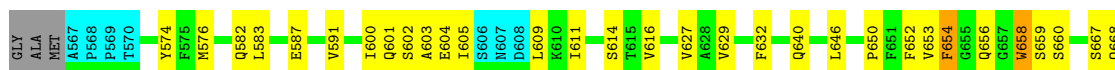


4.2.7 Score per residue for model 7

- Molecule 1: Protein capicua homolog

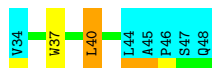


- Molecule 2: Ataxin-1

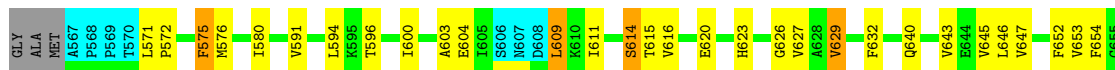


4.2.8 Score per residue for model 8

- Molecule 1: Protein capicua homolog



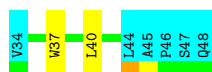
- Molecule 2: Ataxin-1



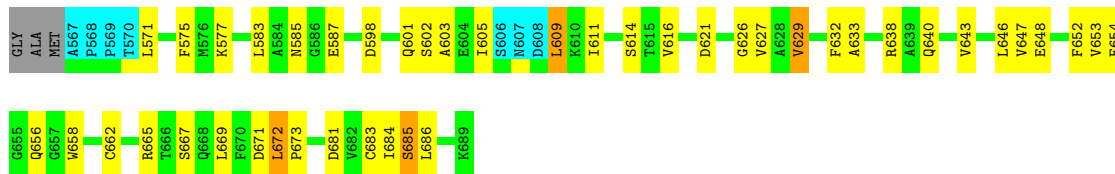
4.2.9 Score per residue for model 9

- Molecule 1: Protein capicua homolog





- Molecule 2: Ataxin-1

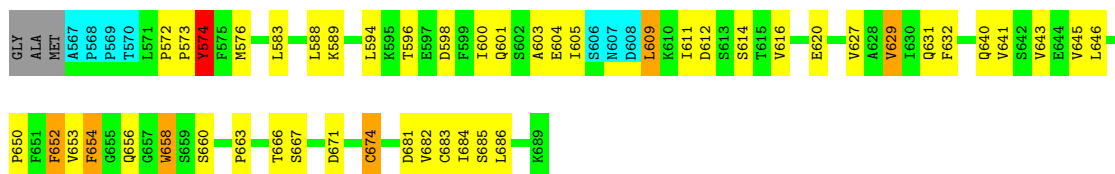


4.2.10 Score per residue for model 10

- Molecule 1: Protein capicua homolog

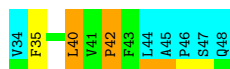
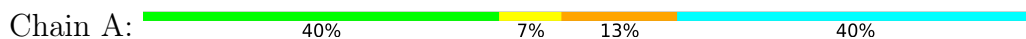


- Molecule 2: Ataxin-1

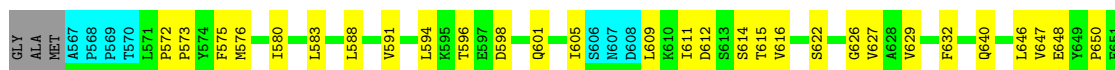


4.2.11 Score per residue for model 11

- Molecule 1: Protein capicua homolog



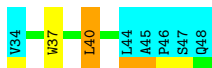
- Molecule 2: Ataxin-1



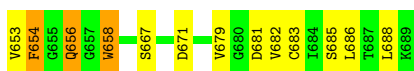


4.2.12 Score per residue for model 12

- Molecule 1: Protein capicua homolog

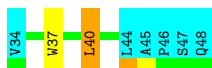


- Molecule 2: Ataxin-1



4.2.13 Score per residue for model 13

- Molecule 1: Protein capicua homolog



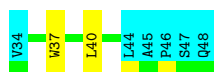
- Molecule 2: Ataxin-1



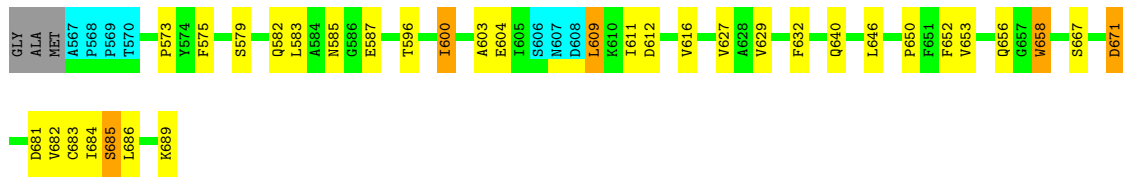
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Protein capicua homolog



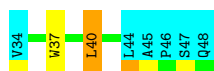


• Molecule 2: Ataxin-1

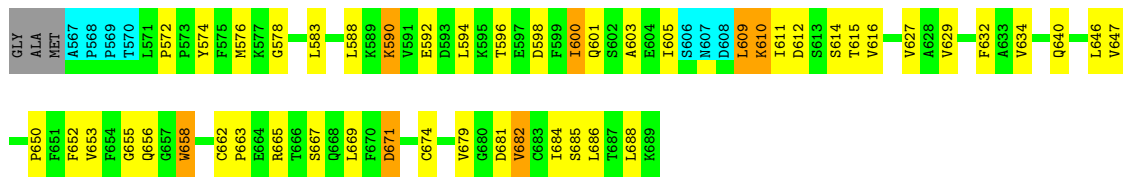


4.2.15 Score per residue for model 15

• Molecule 1: Protein capicua homolog



• Molecule 2: Ataxin-1



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	2.3
ARIA	refinement	2.3

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	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	81	75	74	2±1
2	B	901	902	900	30±4
All	All	14730	14655	14610	455

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:653:VAL:HG12	2:B:656:GLN:HE21	0.88	1.25	13	14
2:B:653:VAL:HG12	2:B:656:GLN:NE2	0.87	1.85	12	15
2:B:653:VAL:HG11	2:B:681:ASP:HB3	0.82	1.50	10	14
2:B:653:VAL:HG11	2:B:681:ASP:HB2	0.78	1.56	7	1
2:B:672:LEU:HD22	2:B:673:PRO:HD2	0.76	1.54	8	2
2:B:666:THR:HB	2:B:674:CYS:SG	0.74	2.22	8	5
2:B:663:PRO:HA	2:B:674:CYS:SG	0.68	2.28	4	5
2:B:632:PHE:O	2:B:640:GLN:HA	0.68	1.89	13	12
2:B:596:THR:O	2:B:600:ILE:HD13	0.67	1.89	14	3
2:B:656:GLN:NE2	2:B:682:VAL:HG13	0.67	2.04	4	6
2:B:616:VAL:HG12	2:B:681:ASP:O	0.67	1.90	6	15
2:B:653:VAL:CG1	2:B:656:GLN:HB2	0.63	2.22	5	8
2:B:600:ILE:O	2:B:604:GLU:HG3	0.62	1.94	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:632:PHE:HE1	2:B:683:CYS:HG	0.62	1.37	1	4
2:B:627:VAL:HG22	2:B:646:LEU:CD2	0.62	2.25	7	14
2:B:650:PRO:HB2	2:B:658:TRP:CH2	0.60	2.31	10	9
2:B:662:CYS:SG	2:B:665:ARG:HB3	0.60	2.36	4	1
2:B:603:ALA:HB3	2:B:611:ILE:HG12	0.60	1.72	13	12
2:B:656:GLN:NE2	2:B:682:VAL:HB	0.60	2.11	5	2
2:B:667:SER:O	2:B:671:ASP:HA	0.60	1.96	11	13
2:B:647:VAL:HB	2:B:662:CYS:SG	0.60	2.37	15	5
1:A:37:TRP:CZ2	2:B:609:LEU:HG	0.59	2.32	9	5
2:B:654:PHE:HB3	2:B:682:VAL:HG13	0.59	1.74	3	5
2:B:672:LEU:HD23	2:B:673:PRO:HD2	0.59	1.74	9	1
2:B:653:VAL:CG1	2:B:681:ASP:HB2	0.59	2.28	7	1
2:B:632:PHE:HE1	2:B:683:CYS:SG	0.58	2.22	3	5
2:B:614:SER:N	2:B:682:VAL:HG23	0.56	2.15	10	9
2:B:601:GLN:O	2:B:605:ILE:HG13	0.56	2.01	13	13
1:A:37:TRP:CZ2	2:B:609:LEU:HD13	0.56	2.36	12	5
2:B:603:ALA:CB	2:B:611:ILE:HG12	0.55	2.31	7	11
2:B:655:GLY:H	2:B:656:GLN:NE2	0.54	2.00	3	2
2:B:665:ARG:O	2:B:669:LEU:HG	0.54	2.02	9	5
2:B:620:GLU:HB2	2:B:629:VAL:HG13	0.54	1.78	5	3
2:B:582:GLN:HA	2:B:587:GLU:O	0.53	2.03	7	6
2:B:653:VAL:CG1	2:B:681:ASP:HB3	0.53	2.33	12	3
2:B:583:LEU:HB3	2:B:602:SER:OG	0.53	2.03	1	7
2:B:572:PRO:HD2	2:B:576:MET:SD	0.53	2.42	6	3
2:B:583:LEU:HD13	2:B:598:ASP:HB3	0.53	1.79	6	3
2:B:583:LEU:HB2	2:B:587:GLU:OE2	0.53	2.03	9	1
2:B:572:PRO:O	2:B:576:MET:HB2	0.52	2.05	10	6
2:B:647:VAL:HG23	2:B:662:CYS:SG	0.52	2.46	4	1
1:A:35:PHE:CD2	2:B:574:TYR:HA	0.51	2.40	10	1
2:B:651:PHE:HD2	2:B:683:CYS:HG	0.50	1.48	12	1
2:B:656:GLN:HE22	2:B:682:VAL:HG13	0.50	1.65	6	6
2:B:572:PRO:HB2	2:B:576:MET:SD	0.50	2.46	10	2
2:B:654:PHE:N	2:B:684:ILE:HG13	0.50	2.20	6	6
2:B:596:THR:OG1	2:B:684:ILE:HD11	0.50	2.07	4	9
2:B:577:LYS:HB2	2:B:671:ASP:O	0.49	2.07	9	1
2:B:573:PRO:O	2:B:579:SER:HB2	0.49	2.07	13	1
2:B:583:LEU:CD1	2:B:598:ASP:HB3	0.49	2.38	6	7
2:B:603:ALA:HB1	2:B:610:LYS:HA	0.49	1.84	13	1
2:B:653:VAL:HB	2:B:656:GLN:HB2	0.49	1.84	3	3
2:B:631:GLN:HA	2:B:641:VAL:O	0.49	2.07	10	3
2:B:577:LYS:HD2	2:B:671:ASP:O	0.49	2.08	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:612:ASP:HB3	2:B:685:SER:HB3	0.48	1.85	4	9
2:B:583:LEU:HD11	2:B:598:ASP:HB3	0.48	1.85	9	3
2:B:648:GLU:HB3	2:B:665:ARG:CD	0.48	2.38	5	1
2:B:612:ASP:HB3	2:B:685:SER:CB	0.48	2.38	14	1
2:B:645:VAL:HG12	2:B:646:LEU:N	0.48	2.23	4	4
2:B:591:VAL:HB	2:B:672:LEU:HD21	0.48	1.85	8	1
2:B:583:LEU:CD1	2:B:598:ASP:HB2	0.48	2.38	10	1
2:B:571:LEU:HD21	2:B:577:LYS:O	0.48	2.09	3	1
2:B:596:THR:HG21	2:B:655:GLY:HA2	0.48	1.86	15	3
2:B:571:LEU:HD11	2:B:577:LYS:O	0.47	2.09	1	1
2:B:575:PHE:O	2:B:672:LEU:HG	0.47	2.10	8	1
2:B:615:THR:HA	2:B:682:VAL:HA	0.47	1.87	15	7
1:A:40:LEU:HD11	2:B:594:LEU:CD1	0.47	2.40	2	9
2:B:653:VAL:HG12	2:B:656:GLN:HB2	0.47	1.87	5	3
1:A:38:HIS:HA	1:A:41:VAL:HG12	0.47	1.86	4	1
2:B:672:LEU:HD22	2:B:673:PRO:CD	0.46	2.35	8	1
2:B:583:LEU:HD12	2:B:587:GLU:HB2	0.46	1.87	5	1
2:B:630:ILE:HB	2:B:632:PHE:CE2	0.46	2.45	1	1
1:A:42:PRO:HD3	2:B:650:PRO:O	0.46	2.11	10	1
2:B:668:GLN:OE1	2:B:668:GLN:HA	0.46	2.11	3	3
2:B:596:THR:HA	2:B:652:PHE:CE1	0.45	2.47	10	2
1:A:37:TRP:CZ2	2:B:609:LEU:HD22	0.45	2.47	15	1
2:B:629:VAL:HA	2:B:643:VAL:O	0.45	2.11	4	6
2:B:614:SER:HB2	2:B:683:CYS:SG	0.45	2.51	9	2
2:B:664:GLU:CD	2:B:664:GLU:H	0.45	2.15	6	1
2:B:653:VAL:HG12	2:B:656:GLN:CD	0.45	2.31	12	1
2:B:626:GLY:O	2:B:646:LEU:HA	0.45	2.12	8	4
2:B:584:ALA:HB3	2:B:602:SER:HA	0.45	1.87	5	1
2:B:576:MET:SD	2:B:576:MET:N	0.45	2.89	10	3
2:B:589:LYS:NZ	2:B:594:LEU:HA	0.45	2.25	10	1
1:A:42:PRO:HG3	2:B:650:PRO:O	0.45	2.11	11	1
2:B:653:VAL:CG1	2:B:656:GLN:HE21	0.45	2.20	3	3
1:A:37:TRP:HA	2:B:581:ILE:CG2	0.45	2.42	1	1
2:B:632:PHE:CE1	2:B:683:CYS:SG	0.45	3.10	10	1
2:B:677:LEU:HD21	2:B:683:CYS:SG	0.45	2.52	7	3
2:B:633:ALA:HB1	2:B:638:ARG:HB3	0.45	1.88	9	1
2:B:654:PHE:HA	2:B:684:ILE:CG1	0.44	2.42	8	2
2:B:612:ASP:CB	2:B:685:SER:HB3	0.44	2.41	12	2
2:B:578:GLY:HA2	2:B:590:LYS:CE	0.44	2.43	13	1
2:B:616:VAL:HG22	2:B:679:VAL:HA	0.44	1.90	11	6
2:B:667:SER:OG	2:B:673:PRO:HA	0.44	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:662:CYS:SG	2:B:662:CYS:O	0.44	2.76	4	1
2:B:583:LEU:HD11	2:B:598:ASP:HB2	0.44	1.90	10	1
2:B:688:LEU:HD22	2:B:688:LEU:N	0.44	2.28	7	2
2:B:610:LYS:NZ	2:B:610:LYS:HB3	0.43	2.27	6	2
1:A:38:HIS:CG	2:B:688:LEU:HD11	0.43	2.47	4	1
2:B:585:ASN:ND2	2:B:587:GLU:HG3	0.43	2.28	12	1
2:B:609:LEU:CD1	2:B:688:LEU:HA	0.43	2.43	11	1
1:A:37:TRP:HZ2	2:B:609:LEU:HD13	0.43	1.73	12	1
2:B:583:LEU:HB2	2:B:585:ASN:OD1	0.43	2.14	5	3
2:B:600:ILE:HD11	2:B:654:PHE:O	0.43	2.13	4	1
2:B:612:ASP:HB2	2:B:685:SER:HB3	0.43	1.89	6	1
2:B:573:PRO:HA	2:B:579:SER:OG	0.43	2.13	6	1
1:A:35:PHE:CZ	2:B:573:PRO:HG2	0.42	2.49	10	3
2:B:676:LYS:HG3	2:B:678:SER:OG	0.42	2.14	11	1
2:B:609:LEU:HD11	2:B:688:LEU:HD13	0.42	1.91	6	1
2:B:576:MET:O	2:B:591:VAL:HG21	0.42	2.15	7	1
2:B:663:PRO:HB3	2:B:674:CYS:O	0.42	2.13	8	2
2:B:615:THR:OG1	2:B:682:VAL:HG22	0.42	2.14	1	2
2:B:578:GLY:N	2:B:590:LYS:HE3	0.42	2.29	4	1
2:B:575:PHE:O	2:B:591:VAL:HG11	0.42	2.14	8	4
1:A:40:LEU:HD13	2:B:591:VAL:HG13	0.42	1.92	1	2
2:B:578:GLY:HA2	2:B:590:LYS:HE3	0.42	1.92	15	1
2:B:632:PHE:CE1	2:B:683:CYS:HB3	0.42	2.49	6	1
2:B:579:SER:HB2	2:B:591:VAL:CG2	0.42	2.44	4	1
1:A:38:HIS:HA	1:A:41:VAL:CG1	0.42	2.45	6	1
2:B:610:LYS:HB2	2:B:687:THR:OG1	0.41	2.15	2	1
2:B:672:LEU:CD2	2:B:673:PRO:HD2	0.41	2.45	5	1
2:B:579:SER:HB3	2:B:591:VAL:CG2	0.41	2.45	1	1
2:B:662:CYS:SG	2:B:664:GLU:HB2	0.41	2.56	6	1
2:B:656:GLN:OE1	2:B:682:VAL:HG12	0.41	2.15	12	1
2:B:581:ILE:HG13	2:B:594:LEU:HD11	0.41	1.92	13	2
2:B:650:PRO:HA	2:B:660:SER:CB	0.41	2.46	7	1
2:B:577:LYS:HG3	2:B:592:GLU:OE2	0.41	2.15	12	1
2:B:590:LYS:O	2:B:594:LEU:HG	0.41	2.15	15	1
2:B:580:ILE:CG2	2:B:588:LEU:HB3	0.41	2.46	11	1
2:B:600:ILE:O	2:B:604:GLU:HG2	0.41	2.16	8	1
2:B:612:ASP:HB3	2:B:685:SER:HB2	0.41	1.92	14	1
2:B:659:SER:OG	2:B:675:SER:HB2	0.40	2.16	7	1
2:B:672:LEU:HD12	2:B:673:PRO:HD2	0.40	1.92	11	1
2:B:585:ASN:HB3	2:B:587:GLU:OE2	0.40	2.16	9	1
2:B:650:PRO:HA	2:B:660:SER:OG	0.40	2.15	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:611:ILE:HG23	2:B:684:ILE:HG23	0.40	1.94	11	1
2:B:573:PRO:O	2:B:579:SER:HB3	0.40	2.16	14	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	9/15 (60%)	7±1 (77±10%)	2±1 (21±10%)	0±0 (1±4%)	14	59
2	B	115/126 (91%)	110±1 (95±1%)	4±2 (4±1%)	1±1 (1±1%)	20	68
All	All	1860/2115 (88%)	1748 (94%)	93 (5%)	19 (1%)	20	68

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	574	TYR	9
2	B	654	PHE	6
1	A	42	PRO	2
2	B	571	LEU	1
2	B	575	PHE	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	9/14 (64%)	8±0 (89±0%)	1±0 (11±0%)	9	53
2	B	104/111 (94%)	97±2 (93±2%)	7±2 (7±2%)	18	66
All	All	1695/1875 (90%)	1568 (93%)	127 (7%)	17	65

All 27 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	40	LEU	15
2	B	629	VAL	15
2	B	652	PHE	15
2	B	658	TRP	15
2	B	686	LEU	15
2	B	682	VAL	7
2	B	609	LEU	6
2	B	674	CYS	5
2	B	671	ASP	5
2	B	575	PHE	4
2	B	648	GLU	3
2	B	600	ILE	3
2	B	571	LEU	2
2	B	672	LEU	2
2	B	610	LYS	2
2	B	685	SER	2
2	B	668	GLN	1
2	B	638	ARG	1
2	B	614	SER	1
2	B	623	HIS	1
2	B	621	ASP	1
2	B	574	TYR	1
2	B	622	SER	1
2	B	656	GLN	1
2	B	590	LYS	1
2	B	592	GLU	1
2	B	688	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 77% 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 [i](#)

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

Total number of shifts	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	26

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	-0.20 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.15 ± 0.31	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	115	-0.38 ± 0.49	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1337 atoms were assigned a chemical shift out of a possible 1696. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	439/616 (71%)	243/249 (98%)	86/250 (34%)	110/117 (94%)
Sidechain	822/924 (89%)	563/606 (93%)	252/295 (85%)	7/23 (30%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	76/156 (49%)	45/77 (58%)	30/71 (42%)	1/8 (12%)
Overall	1337/1696 (79%)	851/932 (91%)	368/616 (60%)	118/148 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1419 atoms were assigned a chemical shift out of a possible 1846. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	469/675 (69%)	264/272 (97%)	90/276 (33%)	115/127 (91%)
Sidechain	874/1015 (86%)	596/666 (89%)	270/324 (83%)	8/25 (32%)
Aromatic	76/156 (49%)	45/77 (58%)	30/71 (42%)	1/8 (12%)
Overall	1419/1846 (77%)	905/1015 (89%)	390/671 (58%)	124/160 (78%)

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	35	PHE	CE2	7.47	124.80 – 136.72	-103.4
1	A	43	PHE	CD2	7.16	125.53 – 137.61	-103.0
1	A	35	PHE	CD2	7.34	125.53 – 137.61	-102.8
1	A	43	PHE	CD1	7.16	125.33 – 137.83	-99.5
1	A	35	PHE	CD1	7.34	125.33 – 137.83	-99.4
1	A	35	PHE	CE1	7.47	124.17 – 137.29	-93.9
1	A	39	SER	CB	3.85	56.28 – 71.32	-39.9
1	A	47	SER	CB	3.91	56.28 – 71.32	-39.8
1	A	48	GLN	CG	2.29	28.36 – 39.21	-29.0
1	A	41	VAL	CG1	0.72	14.71 – 28.29	-15.3
1	A	34	VAL	CG1	0.86	14.71 – 28.29	-15.2
1	A	44	LEU	CD1	0.68	16.71 – 32.55	-15.1
1	A	40	LEU	CD1	0.91	16.71 – 32.55	-15.0
1	A	44	LEU	CD2	0.28	15.73 – 32.47	-14.2
1	A	40	LEU	CD2	0.47	15.73 – 32.47	-14.1
1	A	41	VAL	CG2	0.63	13.71 – 28.88	-13.6
1	A	34	VAL	CG2	0.83	13.71 – 28.88	-13.5
1	A	45	ALA	CB	1.33	10.19 – 27.75	-10.0
1	B	602	SER	HB3	1.47	2.49 – 5.20	-8.8
1	B	657	GLY	HA3	1.57	2.08 – 5.71	-6.4
1	B	650	PRO	HD3	1.34	1.76 – 5.48	-6.1
1	B	652	PHE	HD2	5.22	5.52 – 8.61	-6.0

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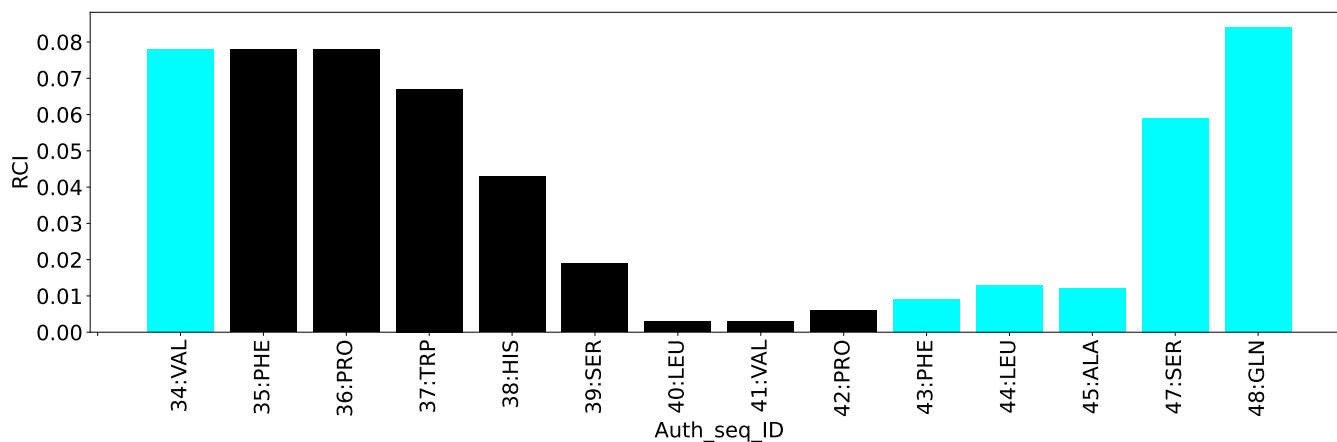
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	652	PHE	HD1	5.22	5.51 – 8.60	-5.9
1	B	575	PHE	HB3	0.78	1.03 – 4.85	-5.7
1	B	650	PRO	HG3	0.13	0.33 – 3.48	-5.6
1	B	650	PRO	HG2	0.33	0.41 – 3.45	-5.3

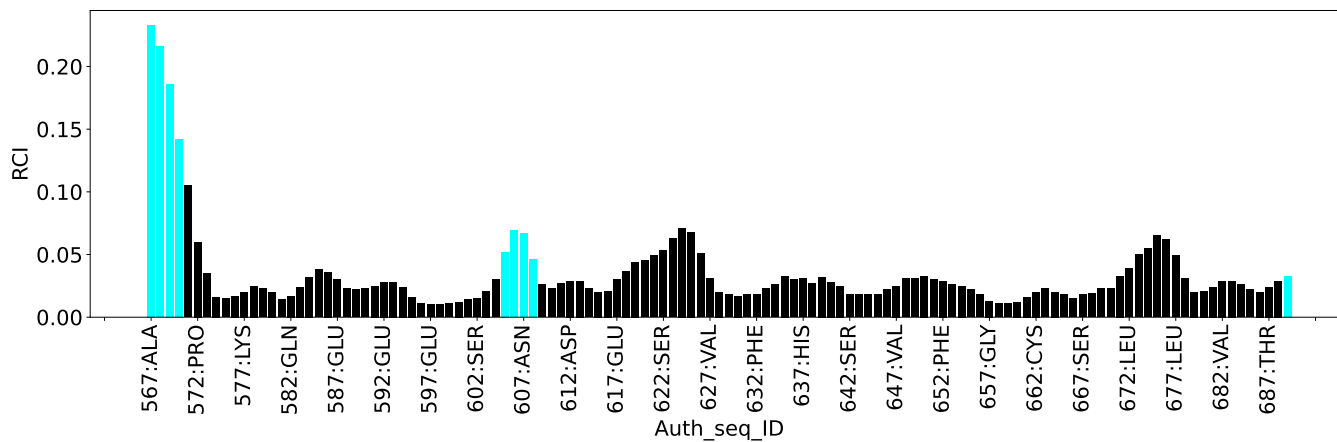
7.1.5 Random Coil Index (RCI) plots [i](#)

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	2986
Intra-residue ($ i-j =0$)	1294
Sequential ($ i-j =1$)	578
Medium range ($ i-j >1$ and $ i-j <5$)	272
Long range ($ i-j \geq 5$)	611
Inter-chain	231
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	21.2
Number of long range restraints per residue ¹	4.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	27.1	0.2
0.2-0.5 (Medium)	44.5	0.5
>0.5 (Large)	63.7	23.03

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis

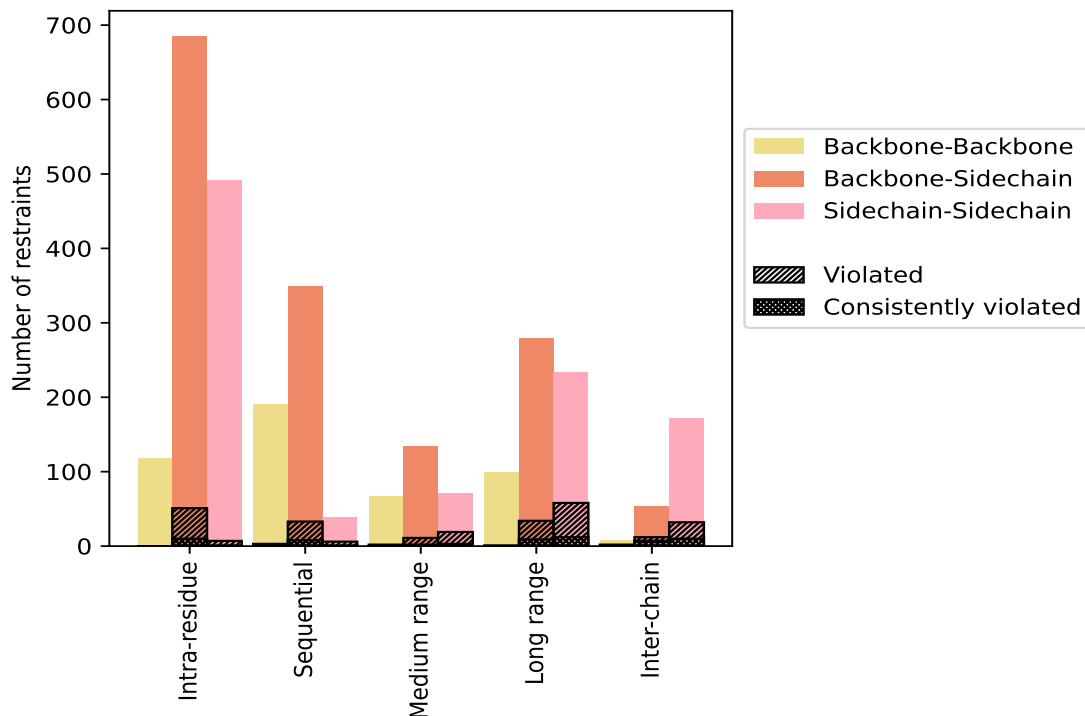
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1294	43.3	58	4.5	1.9	11	0.9	0.4
Backbone-Backbone	118	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	685	22.9	51	7.4	1.7	10	1.5	0.3
Sidechain-Sidechain	491	16.4	7	1.4	0.2	1	0.2	0.0
Sequential ($i-j =1$)	578	19.4	42	7.3	1.4	9	1.6	0.3
Backbone-Backbone	191	6.4	3	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	349	11.7	33	9.5	1.1	8	2.3	0.3
Sidechain-Sidechain	38	1.3	6	15.8	0.2	1	2.6	0.0
Medium range ($i-j >1$ & $i-j <5$)	272	9.1	32	11.8	1.1	5	1.8	0.2
Backbone-Backbone	67	2.2	2	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	134	4.5	11	8.2	0.4	2	1.5	0.1
Sidechain-Sidechain	71	2.4	19	26.8	0.6	3	4.2	0.1
Long range ($i-j \geq 5$)	611	20.5	93	15.2	3.1	21	3.4	0.7
Backbone-Backbone	99	3.3	1	1.0	0.0	0	0.0	0.0
Backbone-Sidechain	279	9.3	34	12.2	1.1	9	3.2	0.3
Sidechain-Sidechain	233	7.8	58	24.9	1.9	12	5.2	0.4
Inter-chain	231	7.7	46	19.9	1.5	17	7.4	0.6
Backbone-Backbone	7	0.2	2	28.6	0.1	0	0.0	0.0
Backbone-Sidechain	53	1.8	12	22.6	0.4	7	13.2	0.2
Sidechain-Sidechain	171	5.7	32	18.7	1.1	10	5.8	0.3
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2986	100.0	271	9.1	9.1	63	2.1	2.1
Backbone-Backbone	482	16.1	8	1.7	0.3	0	0.0	0.0
Backbone-Sidechain	1500	50.2	141	9.4	4.7	36	2.4	1.2
Sidechain-Sidechain	1004	33.6	122	12.2	4.1	27	2.7	0.9

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	25	24	14	50	28	141	0.81	19.01	1.71	0.46
2	22	20	15	44	28	129	0.89	21.51	1.98	0.48
3	26	19	14	38	26	123	0.9	17.55	1.73	0.52
4	25	27	19	49	27	147	0.89	19.43	1.75	0.5
5	22	20	15	54	24	135	0.91	22.09	1.98	0.53
6	18	19	16	45	28	126	0.92	23.03	2.13	0.48
7	25	21	13	47	27	133	0.83	22.24	2.02	0.43
8	23	23	16	49	29	140	0.85	18.93	1.67	0.48
9	25	23	17	50	30	145	0.86	23.03	1.98	0.48
10	25	22	19	44	27	137	0.84	17.44	1.63	0.43
11	23	21	14	45	32	135	0.85	19.46	1.79	0.5

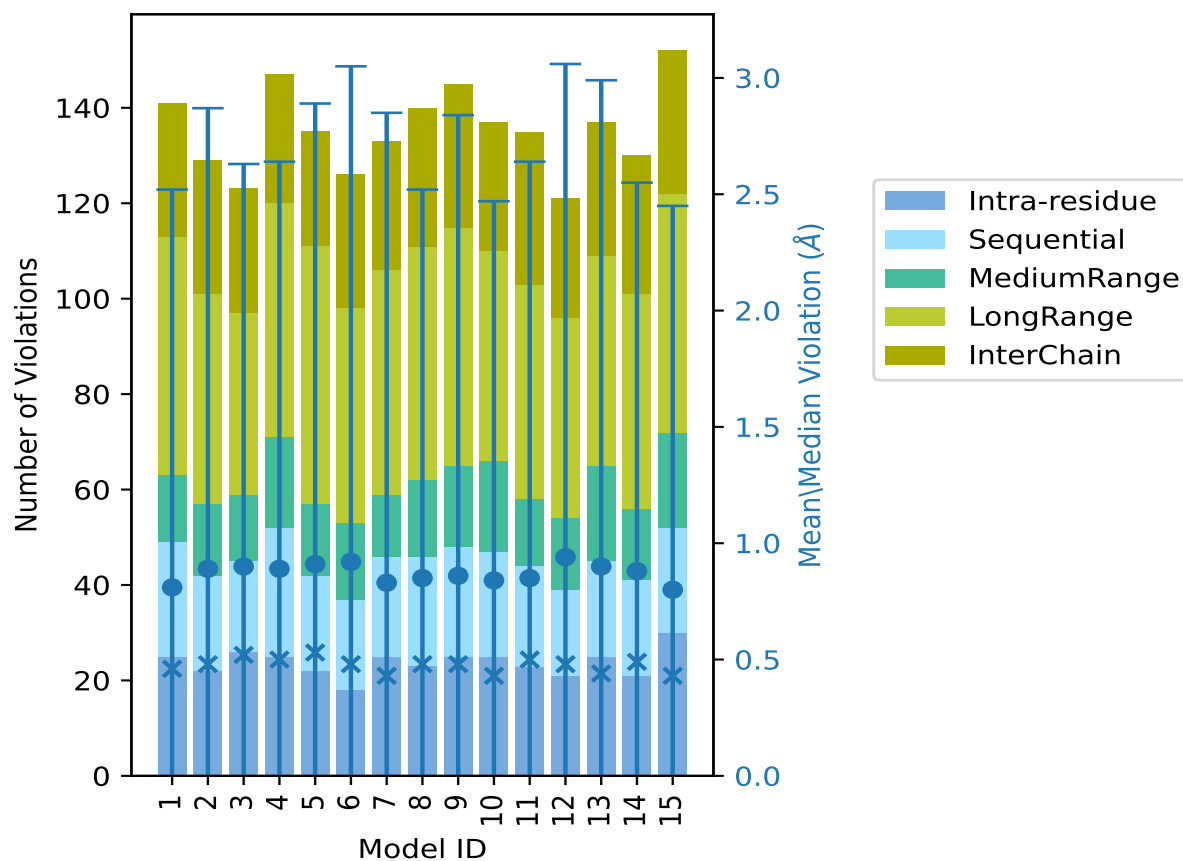
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	21	18	15	42	25	121	0.94	22.28	2.12	0.48
13	25	20	20	44	28	137	0.9	22.74	2.09	0.44
14	21	20	15	45	29	130	0.88	17.13	1.67	0.49
15	30	22	20	50	30	152	0.8	18.84	1.65	0.43

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

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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](#)

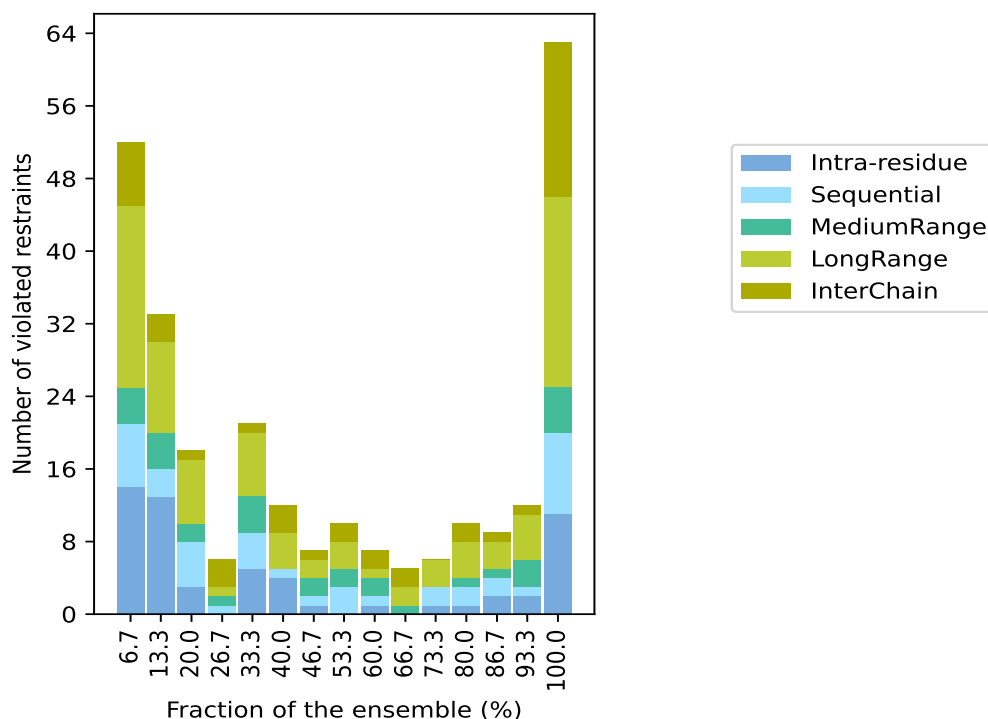
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints

for a given fraction of the ensemble. In total, 2715(IR:1236, SQ:536, MR:240, LR:518, IC:185) 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	%
14	7	4	20	7	52	1	6.7
13	3	4	10	3	33	2	13.3
3	5	2	7	1	18	3	20.0
0	1	1	1	3	6	4	26.7
5	4	4	7	1	21	5	33.3
4	1	0	4	3	12	6	40.0
1	1	2	2	1	7	7	46.7
0	3	2	3	2	10	8	53.3
1	1	2	1	2	7	9	60.0
0	0	1	2	2	5	10	66.7
1	2	0	3	0	6	11	73.3
1	2	1	4	2	10	12	80.0
2	2	1	3	1	9	13	86.7
2	1	3	5	1	12	14	93.3
11	9	5	21	17	63	15	100.0

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

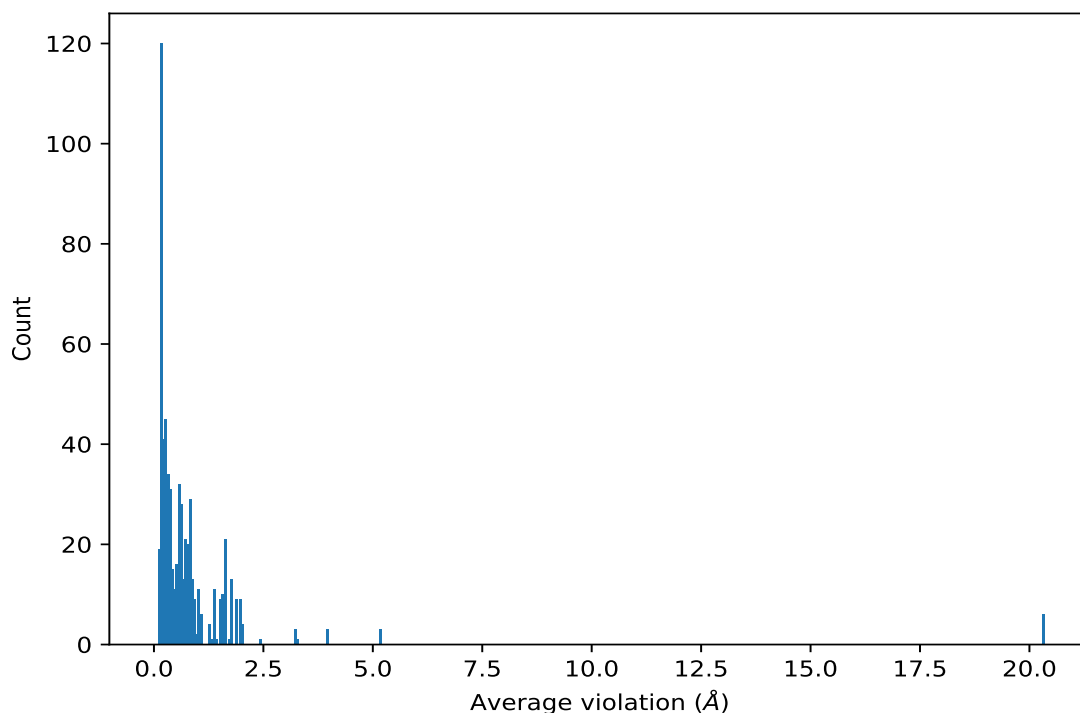
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

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

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



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	15	20.31	2.1	19.46
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	15	20.31	2.1	19.46
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	15	20.31	2.1	19.46
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	15	20.31	2.1	19.46
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	15	20.31	2.1	19.46
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	15	20.31	2.1	19.46
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	15	5.15	0.79	5.31
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	15	5.15	0.79	5.31
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	15	5.15	0.79	5.31
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	15	3.98	0.84	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	15	3.98	0.84	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	15	3.98	0.84	4.11
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	15	3.26	0.26	3.27
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	15	3.2	0.85	3.13
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	15	3.2	0.85	3.13
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	15	3.2	0.85	3.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	15	2.44	0.81	2.38
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	15	2.01	0.25	2.03
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	15	2.01	0.25	2.03
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	15	2.01	0.25	2.03
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	15	2.01	0.25	2.03
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	15	1.95	0.5	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	15	1.95	0.5	2.06
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	15	1.79	0.11	1.76
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	15	1.76	0.6	1.82
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	15	1.76	0.6	1.82
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	15	1.76	0.6	1.82
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	15	1.76	0.6	1.82
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	15	1.76	0.6	1.82
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	15	1.76	0.6	1.82
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	15	1.76	0.6	1.82
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	15	1.74	0.5	1.84
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	15	1.62	0.19	1.6
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	15	1.62	0.19	1.6
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	15	1.62	0.19	1.6
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	15	1.61	0.81	2.1
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	15	1.61	0.81	2.1
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	15	1.6	0.31	1.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	15	1.6	0.31	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	15	1.6	0.31	1.59
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	15	1.59	0.7	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	15	1.59	0.7	1.21
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	15	1.55	0.19	1.57
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	15	1.4	0.41	1.5
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	15	1.39	0.34	1.48
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	15	1.39	0.34	1.48
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	15	1.39	0.34	1.48
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	15	1.37	0.37	1.39
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	15	1.37	0.22	1.43
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	15	1.37	0.22	1.43
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	15	1.37	0.22	1.43
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	15	1.31	0.51	1.38
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	15	1.28	0.05	1.29
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	15	1.08	0.16	1.1
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	15	1.08	0.16	1.1
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	15	1.08	0.16	1.1
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	15	1.03	0.66	0.83
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	15	1.01	0.08	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	15	1.01	0.08	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	15	1.01	0.08	1.03
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	15	1.01	0.08	1.03
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	15	1.01	0.08	1.03
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	15	1.01	0.08	1.03
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	15	0.96	0.05	0.98
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	15	0.95	0.16	0.98
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	15	0.9	0.14	0.92
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	15	0.9	0.14	0.92
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	15	0.9	0.14	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	15	0.87	0.12	0.88
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	15	0.83	0.09	0.83
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	15	0.82	0.14	0.9
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	15	0.82	0.14	0.9
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	15	0.82	0.14	0.9
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	15	0.81	0.24	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	15	0.81	0.24	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	15	0.81	0.24	0.78
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	15	0.81	0.09	0.84
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	15	0.8	0.14	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	15	0.8	0.14	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	15	0.8	0.14	0.82
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	15	0.76	0.08	0.76
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	15	0.75	0.07	0.74
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	15	0.72	0.16	0.72
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	15	0.68	0.06	0.7
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	15	0.66	0.24	0.6
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	15	0.66	0.24	0.6
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	15	0.66	0.24	0.6
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	15	0.66	0.24	0.6
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	15	0.66	0.24	0.6
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	15	0.66	0.24	0.6
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	15	0.63	0.18	0.64
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	15	0.63	0.18	0.64
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	15	0.59	0.14	0.64
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	15	0.59	0.1	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	15	0.59	0.1	0.59
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	15	0.59	0.06	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	15	0.57	0.15	0.53
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	15	0.56	0.1	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	15	0.56	0.1	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	15	0.56	0.1	0.61
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	15	0.52	0.03	0.51
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	15	0.51	0.03	0.51
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	15	0.51	0.05	0.53
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	15	0.39	0.05	0.39
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	15	0.39	0.03	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	15	0.38	0.09	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	15	0.38	0.09	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	15	0.38	0.09	0.4
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	15	0.38	0.12	0.37
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	15	0.37	0.05	0.37
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	15	0.36	0.12	0.36
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	15	0.33	0.03	0.32
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	15	0.33	0.03	0.32
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	15	0.33	0.03	0.32
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	15	0.32	0.11	0.32
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	15	0.32	0.02	0.32
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	15	0.28	0.06	0.29
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	15	0.27	0.1	0.27
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	15	0.27	0.1	0.27
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	15	0.27	0.1	0.27
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	15	0.27	0.1	0.27
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	15	0.27	0.1	0.27
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	15	0.27	0.1	0.27
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	15	0.26	0.15	0.17
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	15	0.26	0.03	0.26
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	15	0.2	0.04	0.21
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	15	0.2	0.04	0.21
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	15	0.17	0.03	0.17
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	15	0.17	0.03	0.17
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	15	0.17	0.03	0.17
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	14	0.78	0.4	0.57
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	14	0.71	0.24	0.8
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	14	0.71	0.24	0.8
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	14	0.5	0.07	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	14	0.5	0.07	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	14	0.5	0.07	0.5
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	14	0.41	0.09	0.42
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	14	0.41	0.09	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	14	0.41	0.09	0.42
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	14	0.26	0.03	0.26
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	14	0.25	0.04	0.25
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	14	0.22	0.09	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	14	0.22	0.09	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	14	0.22	0.09	0.2
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	14	0.22	0.09	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	14	0.2	0.04	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	14	0.2	0.04	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	14	0.2	0.04	0.2
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	14	0.18	0.05	0.16
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	14	0.18	0.05	0.16
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	14	0.18	0.05	0.16
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	14	0.18	0.05	0.16
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	14	0.18	0.05	0.16
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	14	0.18	0.05	0.16
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	14	0.18	0.05	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	14	0.18	0.05	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	14	0.18	0.05	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	14	0.18	0.05	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	14	0.18	0.05	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	14	0.18	0.05	0.15
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	14	0.18	0.04	0.18
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	14	0.18	0.04	0.18
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	14	0.18	0.04	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	14	0.17	0.03	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	14	0.17	0.03	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	14	0.17	0.03	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	14	0.17	0.03	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	14	0.17	0.03	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	14	0.17	0.03	0.18
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	13	1.88	0.87	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	13	1.88	0.87	2.01
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	13	1.01	0.7	0.79
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	13	0.79	0.26	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	13	0.79	0.26	0.81
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	13	0.79	0.26	0.81
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	13	0.73	0.4	0.67
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	13	0.57	0.36	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	13	0.57	0.36	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	13	0.57	0.36	0.4
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	13	0.46	0.05	0.46
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	13	0.34	0.14	0.33
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	13	0.22	0.07	0.22
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	13	0.19	0.05	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	13	0.19	0.05	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	13	0.19	0.05	0.19
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	12	0.76	0.21	0.84
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	12	0.73	0.3	0.74
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	12	0.73	0.3	0.74
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	12	0.65	0.16	0.69
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	12	0.65	0.16	0.69
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	12	0.65	0.16	0.69
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	12	0.44	0.22	0.44
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	12	0.43	0.07	0.41
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	12	0.38	0.06	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	12	0.38	0.06	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	12	0.38	0.06	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	12	0.38	0.06	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	12	0.38	0.06	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	12	0.38	0.06	0.4
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	12	0.37	0.16	0.31
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	12	0.37	0.16	0.31
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	12	0.37	0.16	0.31
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	12	0.24	0.13	0.19
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	12	0.18	0.03	0.18
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	12	0.16	0.02	0.16
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	11	1.36	0.58	1.58
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	11	0.61	0.49	0.37
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	11	0.61	0.49	0.37
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	11	0.61	0.49	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	11	0.38	0.14	0.41
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	11	0.33	0.05	0.33
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	11	0.31	0.14	0.3
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	11	0.31	0.14	0.3
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	11	0.31	0.14	0.3
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	11	0.23	0.05	0.23
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	10	0.64	0.25	0.58
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	10	0.57	0.16	0.5
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	10	0.57	0.16	0.5
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	10	0.57	0.16	0.5
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	10	0.42	0.19	0.4
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	10	0.38	0.11	0.4
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	10	0.38	0.11	0.4
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	10	0.38	0.11	0.4
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	10	0.19	0.05	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	10	0.19	0.05	0.16
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	9	0.91	0.05	0.93
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	9	0.56	0.15	0.63
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	9	0.56	0.15	0.63
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	9	0.49	0.13	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	9	0.49	0.13	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	9	0.49	0.13	0.51
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	9	0.44	0.11	0.46
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	9	0.44	0.11	0.46
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	9	0.44	0.11	0.46
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	9	0.19	0.09	0.15
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	9	0.16	0.05	0.14
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	9	0.16	0.05	0.14
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	9	0.16	0.05	0.14
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	9	0.15	0.02	0.15
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	9	0.15	0.02	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	9	0.15	0.02	0.15
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	9	0.15	0.02	0.15
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	9	0.15	0.02	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	9	0.15	0.02	0.15
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	8	0.34	0.17	0.34
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	8	0.3	0.13	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	8	0.3	0.13	0.3
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	8	0.3	0.13	0.3
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	8	0.25	0.16	0.2
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	8	0.25	0.16	0.2
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	8	0.25	0.16	0.2
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	8	0.25	0.16	0.2
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	8	0.25	0.16	0.2
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	8	0.25	0.16	0.2
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	8	0.24	0.1	0.2
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	8	0.24	0.1	0.2
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	8	0.24	0.1	0.2
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	8	0.24	0.08	0.24
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	8	0.24	0.08	0.24
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	8	0.22	0.04	0.24
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	8	0.21	0.02	0.21
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	8	0.19	0.07	0.17
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	8	0.19	0.07	0.17
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	8	0.19	0.07	0.17
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	8	0.17	0.04	0.17
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	8	0.13	0.01	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	8	0.13	0.01	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	8	0.13	0.01	0.12
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	7	0.41	0.13	0.37
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	7	0.41	0.13	0.37
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	7	0.41	0.13	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	7	0.41	0.13	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	7	0.41	0.13	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	7	0.41	0.13	0.37
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	7	0.38	0.01	0.38
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	7	0.34	0.19	0.33
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	7	0.34	0.19	0.33
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	7	0.33	0.04	0.34
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	7	0.28	0.05	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	7	0.28	0.05	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	7	0.28	0.05	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	7	0.28	0.05	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	7	0.28	0.05	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	7	0.28	0.05	0.26
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	7	0.28	0.21	0.16
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	7	0.18	0.05	0.16
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	7	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	6	0.84	0.37	0.88
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	6	0.84	0.37	0.88
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	6	0.84	0.37	0.88
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	6	0.62	0.02	0.62
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	6	0.62	0.02	0.62
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	6	0.62	0.02	0.62
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	6	0.48	0.16	0.53
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	6	0.38	0.14	0.38
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	6	0.33	0.02	0.32
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	6	0.27	0.08	0.28
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	6	0.25	0.09	0.22
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	6	0.24	0.08	0.22
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	6	0.19	0.06	0.18
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	6	0.17	0.05	0.18
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	6	0.17	0.05	0.18
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	6	0.17	0.05	0.18
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	6	0.15	0.03	0.14
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	6	0.15	0.03	0.14
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	6	0.15	0.03	0.14
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	6	0.12	0.01	0.12
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	5	0.9	0.19	0.88
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	5	0.9	0.19	0.88
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	5	0.87	0.01	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	5	0.87	0.01	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	5	0.87	0.01	0.87
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	5	0.77	0.1	0.77
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	5	0.73	0.24	0.85
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	5	0.73	0.24	0.85
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	5	0.73	0.24	0.85
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	5	0.61	0.45	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	5	0.61	0.45	0.61
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	5	0.56	0.2	0.65
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	5	0.56	0.2	0.65
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	5	0.56	0.2	0.65
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	5	0.45	0.0	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	5	0.39	0.07	0.42
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	5	0.39	0.07	0.42
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	5	0.39	0.07	0.42
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	5	0.37	0.04	0.35
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	5	0.28	0.02	0.28
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	5	0.28	0.02	0.28
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	5	0.28	0.02	0.28
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	5	0.27	0.11	0.24
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	5	0.26	0.11	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	5	0.25	0.12	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	5	0.25	0.12	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	5	0.25	0.12	0.21
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	5	0.25	0.02	0.25
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	5	0.24	0.09	0.19
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	5	0.23	0.06	0.25
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	5	0.18	0.05	0.17
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	5	0.18	0.05	0.17
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	5	0.18	0.05	0.17
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	5	0.18	0.01	0.18
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	5	0.18	0.01	0.18
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	5	0.18	0.01	0.18
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	5	0.16	0.03	0.16
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	5	0.15	0.06	0.13
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	5	0.13	0.01	0.12
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	5	0.13	0.01	0.12
(1,1465)	2:B:580:ILE:H	2:B:579:SER:HB3	4	0.2	0.04	0.19
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB2	4	0.2	0.06	0.17
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB3	4	0.2	0.06	0.17
(1,1298)	2:B:615:THR:HA	2:B:682:VAL:HB	4	0.17	0.01	0.17
(1,2962)	2:B:641:VAL:HG22	1:A:45:ALA:HA	4	0.16	0.04	0.15
(1,2962)	2:B:641:VAL:HG21	1:A:45:ALA:HA	4	0.16	0.04	0.15
(1,2962)	2:B:641:VAL:HG23	1:A:45:ALA:HA	4	0.16	0.04	0.15
(1,2962)	2:B:641:VAL:HG22	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:641:VAL:HG21	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:641:VAL:HG23	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:634:VAL:HG12	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:634:VAL:HG11	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:634:VAL:HG13	1:A:47:SER:HA	4	0.16	0.04	0.15
(1,2962)	2:B:645:VAL:HG22	1:A:44:LEU:HA	4	0.16	0.04	0.15
(1,2962)	2:B:645:VAL:HG21	1:A:44:LEU:HA	4	0.16	0.04	0.15
(1,2962)	2:B:645:VAL:HG23	1:A:44:LEU:HA	4	0.16	0.04	0.15
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG22	4	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG21	4	0.15	0.04	0.15
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG23	4	0.15	0.04	0.15
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG12	4	0.15	0.04	0.15
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG11	4	0.15	0.04	0.15
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG13	4	0.15	0.04	0.15
(1,1240)	2:B:600:ILE:HG12	2:B:597:GLU:HA	4	0.14	0.02	0.15
(1,910)	2:B:672:LEU:HD12	2:B:592:GLU:HB2	3	1.35	0.48	1.09
(1,910)	2:B:672:LEU:HD11	2:B:592:GLU:HB2	3	1.35	0.48	1.09
(1,910)	2:B:672:LEU:HD13	2:B:592:GLU:HB2	3	1.35	0.48	1.09
(1,102)	2:B:672:LEU:HD12	2:B:673:PRO:HD3	3	1.28	0.79	1.62
(1,102)	2:B:672:LEU:HD11	2:B:673:PRO:HD3	3	1.28	0.79	1.62
(1,102)	2:B:672:LEU:HD13	2:B:673:PRO:HD3	3	1.28	0.79	1.62
(1,1102)	2:B:672:LEU:HD22	2:B:666:THR:HA	3	1.09	0.19	1.12
(1,1102)	2:B:672:LEU:HD21	2:B:666:THR:HA	3	1.09	0.19	1.12
(1,1102)	2:B:672:LEU:HD23	2:B:666:THR:HA	3	1.09	0.19	1.12
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD22	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD21	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD23	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD22	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD21	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD23	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD22	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD21	3	0.87	0.3	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD23	3	0.87	0.3	0.97
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD22	3	0.77	0.0	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD21	3	0.77	0.0	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD23	3	0.77	0.0	0.77
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD22	3	0.77	0.04	0.79
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD21	3	0.77	0.04	0.79
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD23	3	0.77	0.04	0.79
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD22	3	0.62	0.02	0.62
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD21	3	0.62	0.02	0.62
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD23	3	0.62	0.02	0.62
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG22	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG21	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG23	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG22	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG21	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG23	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG22	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG21	3	0.54	0.05	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG23	3	0.54	0.05	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2069)	2:B:668:GLN:H	2:B:667:SER:HB3	3	0.46	0.02	0.45
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD22	3	0.34	0.08	0.32
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD21	3	0.34	0.08	0.32
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD23	3	0.34	0.08	0.32
(1,1424)	2:B:571:LEU:H	2:B:570:THR:HA	3	0.27	0.07	0.28
(1,101)	2:B:672:LEU:HD12	2:B:591:VAL:HB	3	0.24	0.06	0.24
(1,101)	2:B:672:LEU:HD11	2:B:591:VAL:HB	3	0.24	0.06	0.24
(1,101)	2:B:672:LEU:HD13	2:B:591:VAL:HB	3	0.24	0.06	0.24
(1,1425)	2:B:571:LEU:H	2:B:571:LEU:HB2	3	0.24	0.09	0.24
(1,2866)	2:B:661:CYS:H	2:B:674:CYS:HB2	3	0.16	0.02	0.17
(1,2866)	2:B:651:PHE:H	2:B:674:CYS:HB2	3	0.16	0.02	0.17
(1,211)	2:B:611:ILE:H	2:B:610:LYS:HB2	3	0.15	0.05	0.12
(1,2956)	2:B:641:VAL:HG12	1:A:44:LEU:HG	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:44:LEU:HG	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:44:LEU:HG	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB2	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB1	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB3	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB2	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB1	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB3	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB2	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB1	3	0.15	0.02	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB3	3	0.15	0.02	0.16
(1,85)	2:B:588:LEU:HD22	2:B:582:GLN:HB3	3	0.12	0.01	0.11
(1,85)	2:B:588:LEU:HD21	2:B:582:GLN:HB3	3	0.12	0.01	0.11
(1,85)	2:B:588:LEU:HD23	2:B:582:GLN:HB3	3	0.12	0.01	0.11
(1,608)	2:B:589:LYS:HE2	2:B:589:LYS:HG3	3	0.11	0.0	0.11
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD22	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD21	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD23	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD22	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD21	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD23	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD22	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD21	2	1.54	0.1	1.54
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD23	2	1.54	0.1	1.54
(1,1255)	2:B:672:LEU:HD12	2:B:592:GLU:HA	2	1.0	0.34	1.0
(1,1255)	2:B:672:LEU:HD11	2:B:592:GLU:HA	2	1.0	0.34	1.0
(1,1255)	2:B:672:LEU:HD13	2:B:592:GLU:HA	2	1.0	0.34	1.0
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD12	2	0.91	0.03	0.91
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD11	2	0.91	0.03	0.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD13	2	0.91	0.03	0.91
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD12	2	0.84	0.36	0.84
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD11	2	0.84	0.36	0.84
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD13	2	0.84	0.36	0.84
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG2	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG2	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG2	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD22	2:B:569:PRO:HB3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD21	2:B:569:PRO:HB3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD23	2:B:569:PRO:HB3	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD22	2:B:572:PRO:HG2	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD21	2:B:572:PRO:HG2	2	0.8	0.13	0.8
(1,2675)	2:B:571:LEU:HD23	2:B:572:PRO:HG2	2	0.8	0.13	0.8
(1,2472)	2:B:686:LEU:HD12	2:B:610:LYS:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD11	2:B:610:LYS:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD13	2:B:610:LYS:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB3	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB3	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB2	2	0.7	0.04	0.7
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB3	2	0.7	0.04	0.7
(1,1168)	2:B:686:LEU:HD12	2:B:609:LEU:HB2	2	0.7	0.24	0.7
(1,1168)	2:B:686:LEU:HD11	2:B:609:LEU:HB2	2	0.7	0.24	0.7
(1,1168)	2:B:686:LEU:HD13	2:B:609:LEU:HB2	2	0.7	0.24	0.7
(1,1269)	2:B:672:LEU:HD22	2:B:575:PHE:HB2	2	0.66	0.4	0.66
(1,1269)	2:B:672:LEU:HD21	2:B:575:PHE:HB2	2	0.66	0.4	0.66
(1,1269)	2:B:672:LEU:HD23	2:B:575:PHE:HB2	2	0.66	0.4	0.66
(1,2530)	2:B:682:VAL:HG22	2:B:613:SER:HB3	2	0.56	0.02	0.56
(1,2530)	2:B:682:VAL:HG21	2:B:613:SER:HB3	2	0.56	0.02	0.56
(1,2530)	2:B:682:VAL:HG23	2:B:613:SER:HB3	2	0.56	0.02	0.56
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG12	2	0.56	0.02	0.56
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG11	2	0.56	0.02	0.56
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG13	2	0.56	0.02	0.56
(1,1454)	2:B:579:SER:H	2:B:579:SER:HB2	2	0.5	0.01	0.5
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG2	2	0.47	0.02	0.47
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG3	2	0.47	0.02	0.47
(1,1773)	2:B:621:ASP:H	2:B:621:ASP:HB3	2	0.46	0.01	0.46
(1,1544)	2:B:590:LYS:H	2:B:590:LYS:HG2	2	0.46	0.32	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,553)	2:B:686:LEU:HD12	2:B:686:LEU:HA	2	0.38	0.02	0.38
(1,553)	2:B:686:LEU:HD11	2:B:686:LEU:HA	2	0.38	0.02	0.38
(1,553)	2:B:686:LEU:HD13	2:B:686:LEU:HA	2	0.38	0.02	0.38
(1,1902)	2:B:640:GLN:H	2:B:640:GLN:HG3	2	0.36	0.01	0.36
(1,2108)	2:B:674:CYS:H	2:B:673:PRO:HB2	2	0.34	0.04	0.34
(1,103)	2:B:672:LEU:HD12	2:B:672:LEU:HA	2	0.32	0.1	0.32
(1,103)	2:B:672:LEU:HD11	2:B:672:LEU:HA	2	0.32	0.1	0.32
(1,103)	2:B:672:LEU:HD13	2:B:672:LEU:HA	2	0.32	0.1	0.32
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG22	2	0.32	0.18	0.32
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG21	2	0.32	0.18	0.32
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG23	2	0.32	0.18	0.32
(1,22)	2:B:571:LEU:HD22	2:B:571:LEU:HA	2	0.28	0.14	0.28
(1,22)	2:B:571:LEU:HD21	2:B:571:LEU:HA	2	0.28	0.14	0.28
(1,22)	2:B:571:LEU:HD23	2:B:571:LEU:HA	2	0.28	0.14	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD12	2	0.28	0.01	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD11	2	0.28	0.01	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD13	2	0.28	0.01	0.28
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD22	2	0.26	0.06	0.26
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD21	2	0.26	0.06	0.26
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD23	2	0.26	0.06	0.26
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD22	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD21	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD23	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD22	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD21	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD23	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD22	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD21	2	0.24	0.01	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD23	2	0.24	0.01	0.24
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD12	2	0.22	0.04	0.22
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD11	2	0.22	0.04	0.22
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD13	2	0.22	0.04	0.22
(1,1417)	1:A:44:LEU:HD12	1:A:45:ALA:H	2	0.18	0.02	0.18
(1,1417)	1:A:44:LEU:HD11	1:A:45:ALA:H	2	0.18	0.02	0.18
(1,1417)	1:A:44:LEU:HD13	1:A:45:ALA:H	2	0.18	0.02	0.18
(1,2029)	2:B:662:CYS:H	2:B:660:SER:HB2	2	0.18	0.05	0.18
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD22	2	0.17	0.06	0.17
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD21	2	0.17	0.06	0.17
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD23	2	0.17	0.06	0.17
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD12	2	0.16	0.04	0.16
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD11	2	0.16	0.04	0.16
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD13	2	0.16	0.04	0.16

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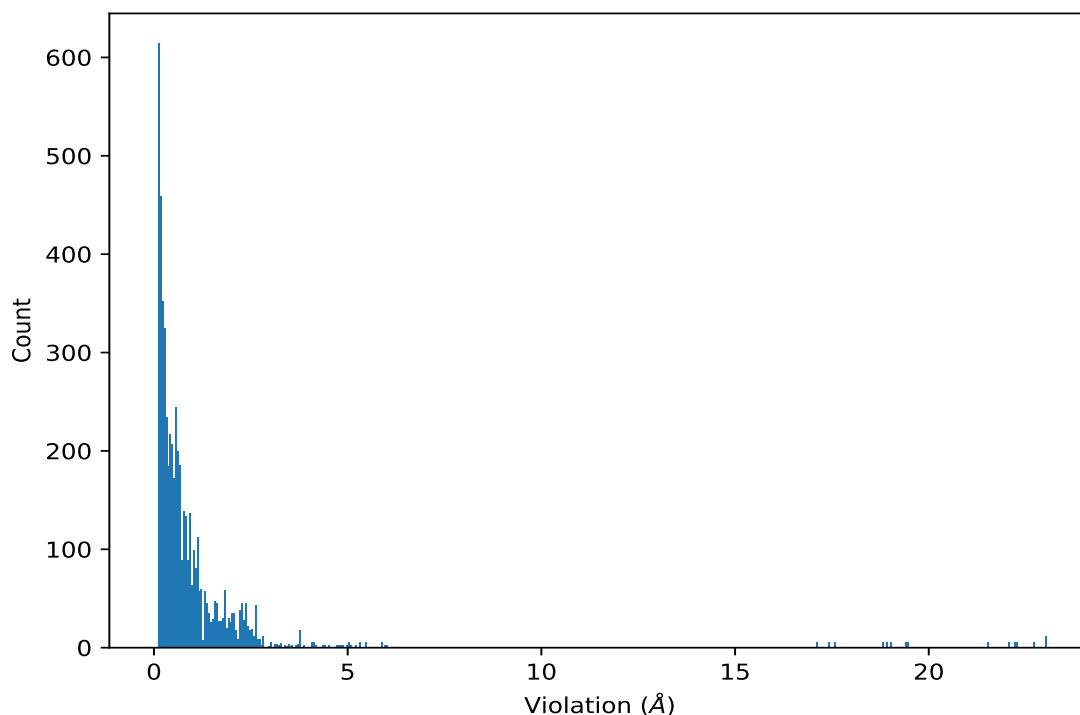
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG22	2	0.16	0.04	0.16
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG21	2	0.16	0.04	0.16
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG23	2	0.16	0.04	0.16
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD12	2	0.16	0.04	0.16
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD11	2	0.16	0.04	0.16
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD13	2	0.16	0.04	0.16
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE2	2	0.16	0.02	0.16
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE3	2	0.16	0.02	0.16
(1,2397)	2:B:629:VAL:HG22	2:B:617:GLU:HA	2	0.16	0.01	0.16
(1,2397)	2:B:629:VAL:HG21	2:B:617:GLU:HA	2	0.16	0.01	0.16
(1,2397)	2:B:629:VAL:HG23	2:B:617:GLU:HA	2	0.16	0.01	0.16
(1,2397)	2:B:629:VAL:HG22	2:B:641:VAL:HA	2	0.16	0.01	0.16
(1,2397)	2:B:629:VAL:HG21	2:B:641:VAL:HA	2	0.16	0.01	0.16
(1,2397)	2:B:629:VAL:HG23	2:B:641:VAL:HA	2	0.16	0.01	0.16
(1,1901)	2:B:640:GLN:H	2:B:640:GLN:HG2	2	0.12	0.02	0.12
(1,441)	2:B:594:LEU:HG	2:B:589:LYS:HA	2	0.12	0.0	0.12
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD12	2	0.11	0.0	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD11	2	0.11	0.0	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD13	2	0.11	0.0	0.11
(1,2643)	2:B:686:LEU:HD22	2:B:686:LEU:HA	2	0.11	0.0	0.11
(1,2643)	2:B:686:LEU:HD21	2:B:686:LEU:HA	2	0.11	0.0	0.11
(1,2643)	2:B:686:LEU:HD23	2:B:686:LEU:HA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	6	23.03
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	6	23.03
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	6	23.03
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	6	23.03
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	6	23.03
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	6	23.03
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	9	23.03
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	9	23.03
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	9	23.03
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	9	23.03
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	9	23.03
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	9	23.03
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	13	22.74
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	13	22.74
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	13	22.74
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	13	22.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	13	22.74
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	13	22.74
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	12	22.28
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	12	22.28
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	12	22.28
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	12	22.28
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	12	22.28
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	12	22.28
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	7	22.24
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	7	22.24
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	7	22.24
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	7	22.24
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	7	22.24
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	7	22.24
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	5	22.09
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	5	22.09
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	5	22.09
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	5	22.09
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	5	22.09
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	5	22.09
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	2	21.51
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	2	21.51
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	2	21.51
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	2	21.51
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	2	21.51
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	2	21.51
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	11	19.46
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	11	19.46
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	11	19.46
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	11	19.46
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	11	19.46
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	11	19.46
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	4	19.43
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	4	19.43
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	4	19.43
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	4	19.43
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	4	19.43
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	4	19.43
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	1	19.01
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	1	19.01
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	1	19.01
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	1	19.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	1	19.01
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	1	19.01
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	8	18.93
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	8	18.93
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	8	18.93
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	8	18.93
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	8	18.93
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	8	18.93
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	15	18.84
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	15	18.84
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	15	18.84
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	15	18.84
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	15	18.84
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	15	18.84
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	3	17.55
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	3	17.55
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	3	17.55
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	3	17.55
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	3	17.55
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	3	17.55
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	10	17.44
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	10	17.44
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	10	17.44
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	10	17.44
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	10	17.44
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	10	17.44
(1,2303)	2:B:567:ALA:HB2	1:A:45:ALA:H	14	17.13
(1,2303)	2:B:567:ALA:HB1	1:A:45:ALA:H	14	17.13
(1,2303)	2:B:567:ALA:HB3	1:A:45:ALA:H	14	17.13
(1,2303)	2:B:567:ALA:HB2	2:B:644:GLU:H	14	17.13
(1,2303)	2:B:567:ALA:HB1	2:B:644:GLU:H	14	17.13
(1,2303)	2:B:567:ALA:HB3	2:B:644:GLU:H	14	17.13
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	13	6.03
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	13	6.03
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	13	6.03
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	4	5.95
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	4	5.95
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	4	5.95
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	3	5.86
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	3	5.86
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	3	5.86
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	7	5.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	7	5.86
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	7	5.86
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	1	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	1	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	1	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	14	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	14	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	14	5.48
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	11	5.34
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	11	5.34
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	11	5.34
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	5	5.31
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	5	5.31
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	5	5.31
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	12	5.24
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	12	5.24
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	12	5.24
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	6	5.08
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	6	5.08
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	6	5.08
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	13	5.01
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	13	5.01
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	13	5.01
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	2	5.0
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	2	5.0
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	2	5.0
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	15	4.99
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	15	4.99
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	15	4.99
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	10	4.87
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	10	4.87
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	10	4.87
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	3	4.84
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	3	4.84
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	3	4.84
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	7	4.75
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	7	4.75
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	7	4.75
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	4	4.71
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	4	4.71
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	4	4.71
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	14	4.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	14	4.52
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	14	4.52
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	11	4.4
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	11	4.4
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	11	4.4
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	13	4.36
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	13	4.36
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	13	4.36
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	14	4.18
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	14	4.18
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	14	4.18
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	1	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	1	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	1	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	5	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	5	4.11
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	5	4.11
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	15	4.09
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	15	4.09
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	15	4.09
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	4	4.06
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	4	4.06
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	4	4.06
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	12	3.89
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	12	3.89
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	12	3.89
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	10	3.79
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	10	3.79
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	10	3.79
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	6	3.78
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	6	3.78
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	6	3.78
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	2	3.76
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	2	3.76
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	2	3.76
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	9	3.75
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	9	3.75
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	9	3.75
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	9	3.75
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	9	3.75
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	9	3.75
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	9	3.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	9	3.75
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	9	3.75
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	15	3.74
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	15	3.74
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	15	3.74
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	14	3.73
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	11	3.66
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	11	3.66
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	11	3.66
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	9	3.56
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	9	3.56
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	9	3.56
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	10	3.55
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	6	3.5
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	13	3.46
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	12	3.45
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	12	3.45
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	12	3.45
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	9	3.44
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	14	3.44
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	1	3.39
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	3	3.39
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	12	3.36
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	3	3.31
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	8	3.29
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	8	3.29
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	8	3.29
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	8	3.29
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	5	3.27
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	7	3.23
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	15	3.2
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	13	3.2
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	12	3.19
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG12	8	3.18
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG11	8	3.18
(1,1363)	1:A:40:LEU:HA	1:A:34:VAL:HG13	8	3.18
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	2	3.13
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	7	3.13
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	7	3.13
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	7	3.13
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	1	3.07
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	5	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	5	3.04
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	5	3.04
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	6	3.03
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	6	3.03
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	6	3.03
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	6	2.97
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	9	2.97
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	4	2.93
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	10	2.83
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	10	2.83
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	10	2.83
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	12	2.81
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	12	2.81
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	12	2.81
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	12	2.81
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	12	2.81
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	12	2.81
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	12	2.81
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	12	2.81
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	12	2.81
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	2	2.8
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	2	2.8
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	2	2.8
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	5	2.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	5	2.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	5	2.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	5	2.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	5	2.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	5	2.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	5	2.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	5	2.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	5	2.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	11	2.68
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	11	2.68
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	11	2.68
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	11	2.68
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	11	2.68
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	11	2.68
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	11	2.68
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	11	2.68
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	11	2.68
(2,12)	2:B:683:CYS:HB2	2:B:656:GLN:HB3	11	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	8	2.63
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	8	2.63
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	8	2.63
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	8	2.63
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	8	2.63
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	8	2.63
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	8	2.63
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	8	2.63
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	8	2.63
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	13	2.63
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	13	2.63
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	13	2.63
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	13	2.63
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	13	2.63
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	13	2.63
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	13	2.63
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	13	2.63
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	13	2.63
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	6	2.63
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	6	2.63
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	6	2.63
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	6	2.63
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	6	2.63
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	6	2.63
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	6	2.63
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	6	2.63
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	6	2.63
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	6	2.63
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	6	2.63
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	6	2.63
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	7	2.62
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	7	2.62
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	7	2.62
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	7	2.62
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	7	2.62
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	7	2.62
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	7	2.62
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	7	2.62
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	7	2.62
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	1	2.61
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	1	2.61
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	1	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	9	2.59
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	9	2.59
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	9	2.59
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	4	2.58
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	4	2.58
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	4	2.58
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	4	2.58
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	4	2.58
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	4	2.58
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	4	2.58
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	4	2.58
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	4	2.58
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	4	2.52
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	10	2.51
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	10	2.51
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	10	2.51
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	10	2.51
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	10	2.51
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	10	2.51
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	10	2.51
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	10	2.51
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	10	2.51
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	4	2.5
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	4	2.5
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	4	2.5
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	4	2.5
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	4	2.5
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	4	2.5
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	4	2.5
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	4	2.5
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	4	2.5
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	3	2.46
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	3	2.46
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	3	2.46
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	3	2.46
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	3	2.46
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	3	2.46
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	3	2.46
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	3	2.46
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	3	2.46
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	15	2.45
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	15	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	15	2.45
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	15	2.45
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	15	2.45
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	15	2.45
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	15	2.45
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	15	2.45
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	15	2.45
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	9	2.42
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	9	2.42
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	9	2.42
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	9	2.42
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	9	2.42
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	9	2.42
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	9	2.42
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	9	2.42
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	9	2.42
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	15	2.42
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	15	2.42
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	15	2.42
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	15	2.42
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	13	2.42
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	13	2.42
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	13	2.42
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	13	2.42
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	13	2.42
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	13	2.42
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	13	2.42
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	13	2.42
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	13	2.42
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	10	2.4
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	11	2.39
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	11	2.39
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	11	2.39
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	11	2.39
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	11	2.39
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	11	2.39
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	11	2.39
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	11	2.39
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	11	2.39
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	11	2.39
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	11	2.39
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	11	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	10	2.38
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	15	2.38
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	15	2.38
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	15	2.38
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	15	2.38
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	15	2.38
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	15	2.38
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	15	2.38
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	15	2.38
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	15	2.38
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	15	2.38
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	15	2.38
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	15	2.38
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	10	2.37
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	14	2.37
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	14	2.37
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	14	2.37
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	14	2.37
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	14	2.37
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	14	2.37
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	14	2.37
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	14	2.37
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	14	2.37
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	11	2.35
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	11	2.35
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	11	2.35
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	11	2.35
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	11	2.35
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	11	2.35
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	11	2.35
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	11	2.35
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	11	2.35
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	2	2.32
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	2	2.32
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	2	2.32
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	2	2.32
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	2	2.32
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	2	2.32
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	2	2.32
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	2	2.32
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	2	2.32
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	5	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	2	2.31
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	2	2.31
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	2	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	2	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	2	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	2	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	2	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	2	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	2	2.31
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	15	2.31
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	15	2.31
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	15	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	15	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	15	2.31
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	15	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	15	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	15	2.31
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	15	2.31
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	12	2.3
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	12	2.3
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	12	2.3
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	12	2.3
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	12	2.3
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	12	2.3
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	12	2.3
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	12	2.3
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	12	2.3
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	3	2.28
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	3	2.28
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	3	2.28
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	3	2.28
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	3	2.28
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	3	2.28
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	3	2.28
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	3	2.28
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	3	2.28
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	8	2.28
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	6	2.27
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	6	2.27
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	6	2.27
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	6	2.27
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	6	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	6	2.27
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	6	2.27
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	6	2.27
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	6	2.27
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	8	2.26
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	8	2.26
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	8	2.26
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	8	2.26
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	9	2.26
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	9	2.26
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	9	2.26
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	11	2.25
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	10	2.25
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	10	2.25
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	10	2.25
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	10	2.25
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	10	2.25
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	10	2.25
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	10	2.25
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	10	2.25
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	10	2.25
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	4	2.24
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	3	2.24
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	3	2.24
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	3	2.24
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	3	2.24
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	3	2.24
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	3	2.24
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	3	2.24
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	3	2.24
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	3	2.24
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	3	2.24
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	3	2.24
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	3	2.24
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	2	2.23
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	10	2.23
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	10	2.23
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	10	2.23
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	10	2.23
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	14	2.23
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	14	2.23
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	14	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	14	2.23
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	13	2.22
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	13	2.22
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	13	2.22
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	13	2.22
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	13	2.22
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	13	2.22
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	13	2.22
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	13	2.22
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	13	2.22
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	13	2.22
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	13	2.22
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	13	2.22
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	2	2.2
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	2	2.2
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	2	2.2
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	2	2.2
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	10	2.19
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	10	2.19
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	10	2.19
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	10	2.19
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	10	2.19
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	10	2.19
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	10	2.19
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	10	2.19
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	10	2.19
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	4	2.12
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	4	2.12
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	4	2.12
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	4	2.12
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	6	2.11
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	6	2.11
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	6	2.11
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	6	2.11
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	8	2.1
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	4	2.1
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	4	2.1
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	4	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	4	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	4	2.1
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	4	2.1
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	4	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	4	2.1
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	4	2.1
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	10	2.08
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	10	2.08
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	10	2.08
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	10	2.08
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	10	2.08
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	10	2.08
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	10	2.08
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	10	2.08
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	10	2.08
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	10	2.08
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	10	2.08
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	10	2.08
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	10	2.08
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	5	2.07
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	13	2.06
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	13	2.06
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	13	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	13	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	13	2.06
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	13	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	13	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	13	2.06
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	13	2.06
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	8	2.06
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	8	2.06
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	8	2.06
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	8	2.06
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	8	2.06
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	8	2.06
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	8	2.06
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	8	2.06
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	8	2.06
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	8	2.06
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	8	2.06
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	8	2.06
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	4	2.05
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	13	2.04
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	13	2.04
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	13	2.04
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	13	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	13	2.04
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	13	2.04
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	13	2.04
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	13	2.04
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	13	2.04
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	13	2.03
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	13	2.03
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	13	2.03
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	13	2.03
(1,102)	2:B:672:LEU:HD12	2:B:673:PRO:HD3	9	2.03
(1,102)	2:B:672:LEU:HD11	2:B:673:PRO:HD3	9	2.03
(1,102)	2:B:672:LEU:HD13	2:B:673:PRO:HD3	9	2.03
(1,910)	2:B:672:LEU:HD12	2:B:592:GLU:HB2	9	2.02
(1,910)	2:B:672:LEU:HD11	2:B:592:GLU:HB2	9	2.02
(1,910)	2:B:672:LEU:HD13	2:B:592:GLU:HB2	9	2.02
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	10	2.02
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	10	2.02
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	10	2.02
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	6	2.01
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	6	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	6	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	6	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	6	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	6	2.01
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	6	2.01
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	6	2.01
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	6	2.01
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG12	8	2.0
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG11	8	2.0
(1,1350)	1:A:40:LEU:HG	1:A:34:VAL:HG13	8	2.0
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	11	1.99
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	11	1.99
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	11	1.99
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	11	1.99
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	2	1.98
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	2	1.98
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	2	1.98
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	5	1.97
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	5	1.97
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	5	1.97
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	5	1.97
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	5	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	5	1.97
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	5	1.97
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	5	1.97
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	5	1.97
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	8	1.96
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	1	1.96
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	1	1.96
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	1	1.96
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	1	1.96
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	1	1.96
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	1	1.96
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	1	1.96
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	1	1.96
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	1	1.96
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	4	1.95
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	4	1.95
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	4	1.95
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	2	1.94
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	14	1.94
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	14	1.94
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	14	1.94
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	14	1.94
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	14	1.94
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	14	1.94
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	14	1.94
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	14	1.94
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	14	1.94
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	13	1.93
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	13	1.93
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	13	1.93
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	14	1.93
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	5	1.92
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	5	1.92
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	5	1.92
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	5	1.92
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	3	1.91
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	3	1.91
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	3	1.91
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	3	1.91
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	3	1.91
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	3	1.91
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	3	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	3	1.91
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	3	1.91
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	6	1.9
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	6	1.9
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	6	1.9
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	6	1.9
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	6	1.9
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	6	1.9
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	6	1.9
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	6	1.9
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	6	1.9
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	14	1.9
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	7	1.89
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	9	1.88
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	7	1.87
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	7	1.87
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	7	1.87
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	7	1.87
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	1	1.86
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	1	1.86
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	1	1.86
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	3	1.85
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	3	1.84
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	4	1.83
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	13	1.83
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	9	1.83
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	15	1.83
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	2	1.82
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	2	1.82
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	2	1.82
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	2	1.82
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	2	1.82
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	2	1.82
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	2	1.82
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	2	1.82
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	2	1.82
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	12	1.82
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	12	1.82
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	12	1.82
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	12	1.82
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	7	1.82
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	7	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	7	1.82
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	7	1.82
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	7	1.82
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	7	1.82
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	7	1.82
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	7	1.82
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	7	1.82
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	7	1.82
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	7	1.82
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	7	1.82
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	1	1.82
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	8	1.82
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	1	1.82
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	6	1.81
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	6	1.81
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	6	1.81
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	6	1.81
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	6	1.81
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	6	1.81
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	6	1.81
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	6	1.81
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	6	1.81
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	12	1.81
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	12	1.81
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	12	1.81
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	12	1.81
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	12	1.81
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	12	1.81
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	12	1.81
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	12	1.81
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	12	1.81
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	12	1.81
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	12	1.81
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	12	1.81
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	9	1.81
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	14	1.81
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	2	1.8
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	5	1.8
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	2	1.79
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	3	1.79
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	3	1.79
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	3	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	13	1.79
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	15	1.79
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	13	1.79
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	11	1.78
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	8	1.78
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	9	1.78
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	14	1.78
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	9	1.77
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	9	1.77
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	9	1.77
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	3	1.77
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	3	1.77
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	3	1.77
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	3	1.77
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	8	1.76
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	10	1.76
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	2	1.76
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	4	1.76
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	12	1.76
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	11	1.75
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	11	1.75
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	11	1.75
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	14	1.75
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	14	1.75
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	14	1.75
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	12	1.75
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	8	1.74
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	8	1.74
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	8	1.74
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	8	1.74
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	8	1.74
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	8	1.74
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	8	1.74
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	8	1.74
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	8	1.74
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	11	1.74
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	1	1.74
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	3	1.74
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	10	1.74
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	10	1.74
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	10	1.74
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	8	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	12	1.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	15	1.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	15	1.72
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	15	1.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	15	1.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	15	1.72
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	15	1.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	15	1.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	15	1.72
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	15	1.72
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	6	1.72
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	12	1.7
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	14	1.7
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	4	1.69
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	7	1.68
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	11	1.68
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	11	1.68
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	13	1.67
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	7	1.67
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	7	1.67
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	7	1.67
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	4	1.67
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	4	1.67
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	4	1.67
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	4	1.67
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	4	1.67
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	4	1.67
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	4	1.67
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	4	1.67
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	4	1.67
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	4	1.67
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	4	1.67
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	4	1.67
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	9	1.66
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	9	1.66
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	9	1.66
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	9	1.66
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	9	1.66
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD22	10	1.65
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD21	10	1.65
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD23	10	1.65
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD22	10	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD21	10	1.65
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD23	10	1.65
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD22	10	1.65
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD21	10	1.65
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD23	10	1.65
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	13	1.65
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	13	1.65
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	13	1.65
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	2	1.65
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	2	1.65
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	2	1.65
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	12	1.64
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	12	1.64
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	12	1.64
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	12	1.64
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	12	1.64
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	12	1.64
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	12	1.64
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	12	1.64
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	12	1.64
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	3	1.64
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	15	1.64
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	14	1.64
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	14	1.64
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	14	1.64
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	8	1.63
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	8	1.63
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	8	1.63
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	6	1.62
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	15	1.62
(1,102)	2:B:672:LEU:HD12	2:B:673:PRO:HD3	5	1.62
(1,102)	2:B:672:LEU:HD11	2:B:673:PRO:HD3	5	1.62
(1,102)	2:B:672:LEU:HD13	2:B:673:PRO:HD3	5	1.62
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	15	1.6
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	12	1.6
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	12	1.6
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	12	1.6
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	9	1.6
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	12	1.6
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	12	1.6
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	12	1.6
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	5	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	13	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	4	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	4	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	4	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	4	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	4	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	4	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	4	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	4	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	4	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	9	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	9	1.59
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	9	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	9	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	9	1.59
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	9	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	9	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	9	1.59
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	9	1.59
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	15	1.59
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	15	1.59
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	15	1.59
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	15	1.59
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	15	1.59
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	15	1.59
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	8	1.58
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	11	1.58
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	8	1.58
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	8	1.58
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	8	1.58
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	8	1.58
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	8	1.58
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	8	1.58
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	8	1.58
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	8	1.58
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	8	1.58
(1,2286)	2:B:659:SER:HA	1:A:40:LEU:HB2	5	1.57
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	6	1.57
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	3	1.57
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	3	1.57
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	3	1.57
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	4	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	2	1.56
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	2	1.56
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	2	1.56
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	10	1.55
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	3	1.54
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	3	1.54
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	3	1.54
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	3	1.54
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	3	1.54
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	3	1.54
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	7	1.54
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	1	1.53
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	1	1.53
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	1	1.53
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	6	1.53
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	6	1.53
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	6	1.52
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	6	1.52
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	6	1.52
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	4	1.52
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	4	1.52
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	4	1.52
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	5	1.51
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	13	1.51
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	2	1.5
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	10	1.5
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	15	1.5
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	15	1.5
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	15	1.5
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	13	1.5
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	13	1.5
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	13	1.5
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	12	1.5
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	1	1.48
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	1	1.48
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	1	1.48
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	1	1.48
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	1	1.48
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	1	1.48
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	1	1.48
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	1	1.48
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	1	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	15	1.48
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	15	1.48
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	15	1.48
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	5	1.48
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	5	1.48
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	5	1.48
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	3	1.47
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	14	1.47
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	14	1.47
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	14	1.47
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	2	1.46
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	2	1.46
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	2	1.46
(1,2952)	2:B:663:PRO:HB2	1:A:40:LEU:HB2	1	1.46
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG2	1	1.46
(1,2952)	2:B:616:VAL:HB	1:A:48:GLN:HG3	1	1.46
(1,2952)	2:B:573:PRO:HB2	1:A:40:LEU:HB2	1	1.46
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	4	1.45
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	7	1.44
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	7	1.44
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	7	1.44
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	7	1.44
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	7	1.44
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	7	1.44
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	7	1.44
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	7	1.44
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	7	1.44
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD22	4	1.44
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD21	4	1.44
(1,322)	2:B:629:VAL:HG22	1:A:44:LEU:HD23	4	1.44
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD22	4	1.44
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD21	4	1.44
(1,322)	2:B:629:VAL:HG21	1:A:44:LEU:HD23	4	1.44
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD22	4	1.44
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD21	4	1.44
(1,322)	2:B:629:VAL:HG23	1:A:44:LEU:HD23	4	1.44
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	9	1.44
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	9	1.44
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	9	1.44
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	6	1.43
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	6	1.43
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	6	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	15	1.42
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	15	1.42
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	15	1.42
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	15	1.42
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	15	1.42
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	15	1.42
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	15	1.42
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	15	1.42
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	15	1.42
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	8	1.41
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	8	1.39
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	8	1.39
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	8	1.39
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	10	1.39
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	10	1.39
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	10	1.39
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	2	1.39
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	2	1.39
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	2	1.39
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	2	1.39
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	2	1.39
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	2	1.39
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	2	1.39
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	2	1.39
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	2	1.39
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	1	1.39
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	2	1.39
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	8	1.39
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	15	1.38
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	1	1.38
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	4	1.38
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	12	1.38
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	10	1.37
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	10	1.37
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	10	1.37
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	10	1.37
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	10	1.37
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	10	1.37
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	10	1.37
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	10	1.37
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	10	1.37
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	9	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG22	5	1.36
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG21	5	1.36
(1,598)	2:B:582:GLN:HB3	2:B:580:ILE:HG23	5	1.36
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	4	1.35
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	13	1.35
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	13	1.35
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	13	1.35
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	13	1.35
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	13	1.35
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	13	1.35
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	13	1.35
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	13	1.35
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	13	1.35
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	12	1.34
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	4	1.34
(1,1255)	2:B:672:LEU:HD12	2:B:592:GLU:HA	9	1.34
(1,1255)	2:B:672:LEU:HD11	2:B:592:GLU:HA	9	1.34
(1,1255)	2:B:672:LEU:HD13	2:B:592:GLU:HA	9	1.34
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	5	1.33
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	14	1.33
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	14	1.33
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	14	1.33
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	14	1.33
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	14	1.33
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	14	1.33
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	14	1.33
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	14	1.33
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	14	1.33
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	5	1.32
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	5	1.32
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	5	1.32
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	5	1.32
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	5	1.32
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	5	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	5	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	5	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	5	1.32
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	14	1.32
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	14	1.32
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	14	1.32
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	14	1.32
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	14	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	14	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	14	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	14	1.32
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	14	1.32
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	11	1.32
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	13	1.32
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	1	1.31
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	6	1.31
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	5	1.31
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	5	1.31
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	5	1.31
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	5	1.31
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	5	1.31
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	5	1.31
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	5	1.31
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	5	1.31
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	5	1.31
(1,799)	2:B:660:SER:HB3	1:A:40:LEU:HA	7	1.3
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	2	1.3
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	4	1.3
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	4	1.3
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	4	1.3
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	3	1.3
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	3	1.3
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	3	1.3
(1,1102)	2:B:672:LEU:HD22	2:B:666:THR:HA	5	1.3
(1,1102)	2:B:672:LEU:HD21	2:B:666:THR:HA	5	1.3
(1,1102)	2:B:672:LEU:HD23	2:B:666:THR:HA	5	1.3
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	14	1.29
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	9	1.27
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	8	1.26
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	15	1.26
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	14	1.25
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	3	1.25
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	3	1.25
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	3	1.25
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	10	1.24
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	11	1.24
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	15	1.24
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	12	1.24
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	12	1.24
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	12	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	12	1.24
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	12	1.24
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	12	1.24
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	12	1.24
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	12	1.24
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	12	1.24
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	2	1.24
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	2	1.24
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	2	1.24
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	2	1.24
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	2	1.24
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	2	1.24
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	2	1.24
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	2	1.24
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	2	1.24
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	2	1.24
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	2	1.24
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	2	1.24
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	12	1.24
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	12	1.24
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	12	1.24
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	3	1.23
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	1	1.23
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	1	1.23
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	1	1.23
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	1	1.23
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	1	1.23
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	1	1.23
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	1	1.23
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	1	1.23
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	1	1.23
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	1	1.23
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	1	1.23
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	1	1.23
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	8	1.23
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	8	1.23
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	8	1.23
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	3	1.22
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	6	1.21
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	6	1.21
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	6	1.21
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	6	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	6	1.21
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	6	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	6	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	6	1.21
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	6	1.21
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	1	1.21
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	1	1.21
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	1	1.21
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	12	1.21
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	12	1.21
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	12	1.21
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD12	10	1.2
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD11	10	1.2
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD13	10	1.2
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	9	1.2
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	9	1.2
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	9	1.2
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	2	1.19
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	2	1.19
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	2	1.19
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	2	1.19
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	2	1.19
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	2	1.19
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	2	1.19
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	2	1.19
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	2	1.19
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	14	1.18
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	1	1.18
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	6	1.18
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	6	1.18
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	6	1.18
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	8	1.18
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	8	1.18
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	8	1.18
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD22	8	1.18
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD21	8	1.18
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD23	8	1.18
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD22	8	1.18
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD21	8	1.18
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD23	8	1.18
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD22	8	1.18
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD21	8	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD23	8	1.18
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	6	1.17
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	11	1.17
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	11	1.17
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	11	1.17
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	11	1.17
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	11	1.17
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	11	1.17
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	11	1.17
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	11	1.17
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	11	1.17
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	2	1.17
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	2	1.17
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	2	1.17
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	2	1.17
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	2	1.17
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	2	1.17
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	2	1.17
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	2	1.17
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	2	1.17
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	11	1.17
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	11	1.17
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	11	1.17
(1,639)	2:B:658:TRP:HB3	2:B:593:ASP:HA	7	1.16
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	14	1.16
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	14	1.16
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG12	9	1.15
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG11	9	1.15
(1,893)	2:B:630:ILE:HD12	2:B:645:VAL:HG13	9	1.15
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG12	9	1.15
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG11	9	1.15
(1,893)	2:B:630:ILE:HD11	2:B:645:VAL:HG13	9	1.15
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG12	9	1.15
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG11	9	1.15
(1,893)	2:B:630:ILE:HD13	2:B:645:VAL:HG13	9	1.15
(1,850)	2:B:679:VAL:HG22	2:B:617:GLU:HA	4	1.15
(1,850)	2:B:679:VAL:HG21	2:B:617:GLU:HA	4	1.15
(1,850)	2:B:679:VAL:HG23	2:B:617:GLU:HA	4	1.15
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	11	1.15
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	11	1.15
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	11	1.15
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	7	1.14
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	7	1.14
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	7	1.14
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	7	1.14
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	7	1.14
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	15	1.14
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	15	1.14
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	15	1.14
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	9	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	1	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	1	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	1	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	1	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	1	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	1	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	1	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	1	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	1	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	3	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	3	1.13
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	3	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	3	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	3	1.13
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	3	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	3	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	3	1.13
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	3	1.13
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	12	1.13
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	12	1.13
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	5	1.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	5	1.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	5	1.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	5	1.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	5	1.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	5	1.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	5	1.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	5	1.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	5	1.12
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	5	1.12
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	8	1.12
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	8	1.12
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	8	1.12
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	8	1.12
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	8	1.12
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	14	1.12
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	14	1.12
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	14	1.12
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	14	1.12
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	14	1.12
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	14	1.12
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	14	1.12
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	14	1.12
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	14	1.12
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	14	1.12
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	14	1.12
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	14	1.12
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	2	1.12
(1,1102)	2:B:672:LEU:HD22	2:B:666:THR:HA	8	1.12
(1,1102)	2:B:672:LEU:HD21	2:B:666:THR:HA	8	1.12
(1,1102)	2:B:672:LEU:HD23	2:B:666:THR:HA	8	1.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	8	1.11
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	8	1.11
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	8	1.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	8	1.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	8	1.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	8	1.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	8	1.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	8	1.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	8	1.11
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	8	1.11
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	8	1.11
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	8	1.11
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	8	1.11
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	8	1.11
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	8	1.11
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	8	1.11
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	8	1.11
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	8	1.11
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	9	1.11
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	2	1.11
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	2	1.11
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	2	1.11
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	1	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	1	1.11
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	1	1.11
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	12	1.11
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	12	1.11
(1,1934)	2:B:679:VAL:H	2:B:679:VAL:HG12	4	1.1
(1,1934)	2:B:679:VAL:H	2:B:679:VAL:HG11	4	1.1
(1,1934)	2:B:679:VAL:H	2:B:679:VAL:HG13	4	1.1
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	6	1.1
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	6	1.1
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	14	1.1
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	14	1.1
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	14	1.1
(1,910)	2:B:672:LEU:HD12	2:B:592:GLU:HB2	5	1.09
(1,910)	2:B:672:LEU:HD11	2:B:592:GLU:HB2	5	1.09
(1,910)	2:B:672:LEU:HD13	2:B:592:GLU:HB2	5	1.09
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	11	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	1	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	1	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	1	1.09
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	1	1.09
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	1	1.09
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	1	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	9	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	9	1.09
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	9	1.09
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	9	1.09
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	9	1.09
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	9	1.09
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	5	1.09
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	5	1.09
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	5	1.09
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	13	1.09
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	13	1.09
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	13	1.09
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	13	1.09
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	13	1.08
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	13	1.08
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	13	1.08
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	11	1.08
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	11	1.08
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	11	1.08
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	11	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	11	1.08
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	11	1.08
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	15	1.08
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	5	1.08
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	5	1.08
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	5	1.08
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	13	1.07
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	13	1.07
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	13	1.07
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	13	1.07
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	13	1.07
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	13	1.07
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	13	1.07
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	13	1.07
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	13	1.07
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	14	1.07
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	4	1.07
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	4	1.07
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	4	1.07
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	4	1.07
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	4	1.07
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	4	1.07
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	4	1.06
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	15	1.06
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	4	1.06
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	4	1.06
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	4	1.06
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	4	1.06
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	4	1.06
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	4	1.06
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	1	1.05
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD22	7	1.05
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD21	7	1.05
(1,563)	2:B:688:LEU:HD12	2:B:583:LEU:HD23	7	1.05
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD22	7	1.05
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD21	7	1.05
(1,563)	2:B:688:LEU:HD11	2:B:583:LEU:HD23	7	1.05
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD22	7	1.05
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD21	7	1.05
(1,563)	2:B:688:LEU:HD13	2:B:583:LEU:HD23	7	1.05
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	3	1.05
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	3	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	3	1.05
(1,2204)	2:B:616:VAL:HG12	1:A:44:LEU:HB2	8	1.05
(1,2204)	2:B:616:VAL:HG11	1:A:44:LEU:HB2	8	1.05
(1,2204)	2:B:616:VAL:HG13	1:A:44:LEU:HB2	8	1.05
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	1	1.05
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	5	1.05
(1,1269)	2:B:672:LEU:HD22	2:B:575:PHE:HB2	9	1.05
(1,1269)	2:B:672:LEU:HD21	2:B:575:PHE:HB2	9	1.05
(1,1269)	2:B:672:LEU:HD23	2:B:575:PHE:HB2	9	1.05
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	13	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	7	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	7	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	7	1.04
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	7	1.04
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	7	1.04
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	7	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	15	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	15	1.04
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	15	1.04
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	15	1.04
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	15	1.04
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	15	1.04
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	7	1.04
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	7	1.04
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	7	1.04
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	7	1.04
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	7	1.04
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	7	1.04
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	7	1.04
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	7	1.04
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	7	1.04
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	10	1.03
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	10	1.03
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	10	1.03
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	10	1.03
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	10	1.03
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	10	1.03
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	10	1.03
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	10	1.03
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	10	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	5	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	5	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	5	1.03
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	5	1.03
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	5	1.03
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	5	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	12	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	12	1.03
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	12	1.03
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	12	1.03
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	12	1.03
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	12	1.03
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	3	1.03
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	11	1.03
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	11	1.03
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	11	1.03
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	9	1.03
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	9	1.03
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	9	1.03
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	5	1.02
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	5	1.01
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	5	1.01
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	5	1.01
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	5	1.01
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	5	1.01
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	5	1.01
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	5	1.01
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	5	1.01
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	5	1.01
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	5	1.01
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	5	1.01
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	5	1.01
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	14	1.01
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	14	1.01
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	14	1.01
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	14	1.01
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	14	1.01
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	14	1.01
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	14	1.01
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	14	1.01
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	14	1.01
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	7	1.01
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	7	1.01
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	15	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	15	1.01
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	10	1.0
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	9	1.0
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	9	1.0
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	9	1.0
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	9	1.0
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	9	1.0
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	9	1.0
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	9	1.0
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	9	1.0
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	9	1.0
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	2	1.0
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	2	1.0
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	2	1.0
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	2	1.0
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	2	1.0
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	2	1.0
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	2	1.0
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	2	1.0
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	2	1.0
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	3	1.0
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	6	1.0
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	6	1.0
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	6	1.0
(1,489)	2:B:674:CYS:HB3	2:B:663:PRO:HB2	6	0.99
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	14	0.99
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	14	0.99
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	14	0.99
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	14	0.99
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	14	0.99
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	14	0.99
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	12	0.99
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	2	0.99
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	7	0.99
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	11	0.99
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	12	0.99
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	13	0.99
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	8	0.99
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	10	0.99
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	13	0.99
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	13	0.99
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	13	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	12	0.98
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	3	0.98
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	3	0.98
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	3	0.98
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	3	0.98
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	3	0.98
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	3	0.98
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	3	0.98
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	3	0.98
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	3	0.98
(1,2207)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	5	0.98
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	5	0.98
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	6	0.98
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	15	0.97
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	15	0.97
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	15	0.97
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	6	0.97
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	6	0.97
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	6	0.97
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	6	0.97
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	6	0.97
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	6	0.97
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	13	0.97
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	13	0.97
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD22	5	0.97
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD21	5	0.97
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD23	5	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD22	5	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD21	5	0.97
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD23	5	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD22	5	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD21	5	0.97
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD23	5	0.97
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	2	0.96
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	2	0.96
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	2	0.96
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	15	0.96
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	7	0.96
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	12	0.96
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	12	0.96
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	12	0.96
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	13	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	10	0.96
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	2	0.96
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	2	0.96
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	2	0.96
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	3	0.95
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	3	0.95
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	3	0.95
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	10	0.95
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	10	0.95
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	10	0.95
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	9	0.95
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	5	0.95
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	4	0.95
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	11	0.95
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	8	0.95
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	7	0.95
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	7	0.95
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	7	0.95
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	9	0.95
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	9	0.95
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	9	0.95
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	11	0.94
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	12	0.94
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	12	0.94
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	12	0.94
(1,910)	2:B:672:LEU:HD12	2:B:592:GLU:HB2	8	0.94
(1,910)	2:B:672:LEU:HD11	2:B:592:GLU:HB2	8	0.94
(1,910)	2:B:672:LEU:HD13	2:B:592:GLU:HB2	8	0.94
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	9	0.94
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD12	8	0.94
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD11	8	0.94
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD13	8	0.94
(1,516)	2:B:679:VAL:HG12	2:B:678:SER:HA	4	0.94
(1,516)	2:B:679:VAL:HG11	2:B:678:SER:HA	4	0.94
(1,516)	2:B:679:VAL:HG13	2:B:678:SER:HA	4	0.94
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	15	0.94
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	3	0.94
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	3	0.94
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	13	0.94
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	13	0.94
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	13	0.94
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	8	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	8	0.94
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	3	0.94
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	6	0.94
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	15	0.94
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	1	0.94
(1,1168)	2:B:686:LEU:HD12	2:B:609:LEU:HB2	1	0.94
(1,1168)	2:B:686:LEU:HD11	2:B:609:LEU:HB2	1	0.94
(1,1168)	2:B:686:LEU:HD13	2:B:609:LEU:HB2	1	0.94
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	6	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	6	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	6	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	15	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	15	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	15	0.93
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG2	9	0.93
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG3	9	0.93
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG2	9	0.93
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG3	9	0.93
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG2	9	0.93
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG3	9	0.93
(1,2675)	2:B:571:LEU:HD22	2:B:569:PRO:HB3	9	0.93
(1,2675)	2:B:571:LEU:HD21	2:B:569:PRO:HB3	9	0.93
(1,2675)	2:B:571:LEU:HD23	2:B:569:PRO:HB3	9	0.93
(1,2675)	2:B:571:LEU:HD22	2:B:572:PRO:HG2	9	0.93
(1,2675)	2:B:571:LEU:HD21	2:B:572:PRO:HG2	9	0.93
(1,2675)	2:B:571:LEU:HD23	2:B:572:PRO:HG2	9	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	3	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	3	0.93
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	3	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	10	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	10	0.93
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	10	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	12	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	12	0.93
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	12	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	14	0.93
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	14	0.93
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	14	0.93
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	3	0.93
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	3	0.93
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	3	0.93
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	3	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	3	0.93
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	3	0.93
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	12	0.93
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	12	0.93
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	12	0.93
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	12	0.93
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	12	0.93
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	12	0.93
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	12	0.93
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	12	0.93
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	12	0.93
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	10	0.93
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	11	0.93
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	4	0.93
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	3	0.93
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	9	0.92
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	9	0.92
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	9	0.92
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	11	0.92
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	4	0.92
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	4	0.92
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	4	0.92
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	9	0.92
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	9	0.92
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	9	0.92
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	2	0.92
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	14	0.92
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	4	0.91
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	8	0.91
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	8	0.91
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	8	0.91
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	8	0.91
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	8	0.91
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	8	0.91
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	8	0.91
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	8	0.91
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	8	0.91
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	8	0.91
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	10	0.91
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	15	0.91
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	1	0.91
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	11	0.91
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	11	0.91
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	2	0.91
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	11	0.9
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	11	0.9
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	11	0.9
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	5	0.9
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	5	0.9
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	5	0.9
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	7	0.9
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	7	0.9
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	7	0.9
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	6	0.9
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	1	0.9
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	8	0.9
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	2	0.89
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	5	0.89
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	5	0.89
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	5	0.89
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	7	0.89
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	7	0.89
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	9	0.89
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	9	0.89
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	9	0.89
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	9	0.89
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	9	0.89
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	9	0.89
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	9	0.89
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	9	0.89
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	9	0.89
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	9	0.89
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	9	0.89
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	9	0.89
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	10	0.89
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	12	0.89
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	12	0.89
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	12	0.89
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	8	0.88
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	10	0.88
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	13	0.88
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	13	0.88
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	13	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	6	0.88
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	7	0.88
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	7	0.88
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	7	0.88
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD12	1	0.88
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD11	1	0.88
(1,556)	2:B:687:THR:H	2:B:686:LEU:HD13	1	0.88
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	11	0.88
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	11	0.88
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	11	0.88
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	7	0.88
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	4	0.88
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	4	0.88
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	4	0.88
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	13	0.88
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	4	0.88
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	15	0.88
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	15	0.88
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	5	0.88
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	14	0.88
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	14	0.88
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	14	0.88
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD22	4	0.87
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD21	4	0.87
(1,564)	2:B:688:LEU:HD22	2:B:583:LEU:HD23	4	0.87
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD22	4	0.87
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD21	4	0.87
(1,564)	2:B:688:LEU:HD21	2:B:583:LEU:HD23	4	0.87
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD22	4	0.87
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD21	4	0.87
(1,564)	2:B:688:LEU:HD23	2:B:583:LEU:HD23	4	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	1	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	1	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	1	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	5	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	5	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	5	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	14	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	14	0.87
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	14	0.87
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	10	0.87
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	13	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	10	0.87
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	5	0.87
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	3	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	5	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	5	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	5	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	14	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	14	0.86
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	14	0.86
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	14	0.86
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG12	2	0.86
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG11	2	0.86
(1,2161)	2:B:682:VAL:H	2:B:682:VAL:HG13	2	0.86
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	8	0.86
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	3	0.86
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	6	0.86
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	12	0.86
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	15	0.86
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	15	0.86
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	15	0.86
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	6	0.85
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	8	0.85
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	9	0.85
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	9	0.85
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	9	0.85
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	11	0.85
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	1	0.85
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	1	0.85
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	1	0.85
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	1	0.85
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	1	0.85
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	1	0.85
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	1	0.85
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	1	0.85
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	1	0.85
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	10	0.85
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	10	0.85
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	10	0.85
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	10	0.85
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	10	0.85
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	10	0.85
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	9	0.85
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	14	0.85
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	15	0.85
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	10	0.85
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	12	0.85
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	1	0.85
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	1	0.85
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	1	0.85
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	7	0.84
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	11	0.84
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	6	0.84
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	6	0.84
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	6	0.84
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	4	0.84
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	6	0.84
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	6	0.84
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	6	0.84
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	6	0.84
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	6	0.84
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	6	0.84
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	6	0.84
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	6	0.84
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	6	0.84
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	6	0.84
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	6	0.84
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	6	0.84
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	9	0.84
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	8	0.84
(1,1102)	2:B:672:LEU:HD22	2:B:666:THR:HA	9	0.84
(1,1102)	2:B:672:LEU:HD21	2:B:666:THR:HA	9	0.84
(1,1102)	2:B:672:LEU:HD23	2:B:666:THR:HA	9	0.84
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	8	0.83
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	7	0.83
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	4	0.83
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	4	0.83
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	4	0.83
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	4	0.83
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	4	0.83
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	4	0.83
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	4	0.83
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	4	0.83
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	4	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	11	0.83
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	8	0.83
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	15	0.83
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	15	0.83
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	10	0.83
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD12	13	0.82
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD11	13	0.82
(1,2549)	2:B:649:TYR:HA	1:A:40:LEU:HD13	13	0.82
(1,2549)	2:B:647:VAL:HG12	2:B:649:TYR:HA	13	0.82
(1,2549)	2:B:647:VAL:HG11	2:B:649:TYR:HA	13	0.82
(1,2549)	2:B:647:VAL:HG13	2:B:649:TYR:HA	13	0.82
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	12	0.82
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	7	0.82
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	7	0.82
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	7	0.82
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	2	0.82
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	14	0.82
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	14	0.82
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	7	0.82
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	8	0.82
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	11	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	1	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	1	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	1	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	3	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	3	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	3	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	7	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	7	0.82
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	7	0.82
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	6	0.81
(1,243)	2:B:616:VAL:HG12	2:B:631:GLN:HE22	3	0.81
(1,243)	2:B:616:VAL:HG11	2:B:631:GLN:HE22	3	0.81
(1,243)	2:B:616:VAL:HG13	2:B:631:GLN:HE22	3	0.81
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	8	0.81
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	8	0.81
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	8	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	8	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	8	0.81
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	8	0.81
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	8	0.81
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	8	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	8	0.81
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	7	0.81
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	2	0.81
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	5	0.81
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	14	0.81
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD22	15	0.81
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD21	15	0.81
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD23	15	0.81
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	2	0.8
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	15	0.8
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	15	0.8
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	15	0.8
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	15	0.8
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	15	0.8
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	15	0.8
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	15	0.8
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	15	0.8
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	15	0.8
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	1	0.8
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	1	0.8
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	1	0.8
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	4	0.8
(1,2143)	2:B:680:GLY:H	2:B:679:VAL:HG22	4	0.8
(1,2143)	2:B:680:GLY:H	2:B:679:VAL:HG21	4	0.8
(1,2143)	2:B:680:GLY:H	2:B:679:VAL:HG23	4	0.8
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	3	0.8
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	8	0.8
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	8	0.8
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	14	0.79
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	1	0.79
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	1	0.79
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	1	0.79
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	2	0.79
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	5	0.79
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	5	0.79
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	5	0.79
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	5	0.79
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	9	0.79
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	9	0.79
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	9	0.79
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	6	0.79
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	6	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	3	0.79
(1,1429)	2:B:576:MET:H	2:B:575:PHE:HZ	9	0.79
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	3	0.79
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD22	5	0.79
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD21	5	0.79
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD23	5	0.79
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	6	0.79
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	6	0.79
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	6	0.79
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	2	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	2	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	2	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	4	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	4	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	4	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	13	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	13	0.78
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	13	0.78
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	5	0.78
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	5	0.78
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	5	0.78
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	5	0.78
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	5	0.78
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	5	0.78
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	5	0.78
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	5	0.78
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	5	0.78
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	3	0.78
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	2	0.78
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	2	0.78
(1,1518)	2:B:587:GLU:H	2:B:587:GLU:HB2	9	0.78
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD22	4	0.78
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD21	4	0.78
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD23	4	0.78
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	4	0.78
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	5	0.77
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	12	0.77
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	12	0.77
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	12	0.77
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	12	0.77
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	12	0.77
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	12	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	12	0.77
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	12	0.77
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	12	0.77
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	9	0.77
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	11	0.77
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	8	0.77
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	11	0.77
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	11	0.77
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	11	0.77
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	11	0.77
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	11	0.77
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	11	0.77
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	11	0.77
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	11	0.77
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	11	0.77
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	15	0.77
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	15	0.77
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	15	0.77
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	15	0.77
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	15	0.77
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	15	0.77
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	15	0.77
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	15	0.77
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	15	0.77
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	4	0.77
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	4	0.77
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	4	0.77
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	1	0.77
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	6	0.77
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	2	0.77
(1,1544)	2:B:590:LYS:H	2:B:590:LYS:HG2	9	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD22	5	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD21	5	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD23	5	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD22	15	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD21	15	0.77
(1,1220)	2:B:677:LEU:HA	2:B:677:LEU:HD23	15	0.77
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	4	0.77
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	4	0.77
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	4	0.77
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	1	0.76
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	1	0.76
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	12	0.76
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	12	0.76
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	12	0.76
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	11	0.76
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	11	0.76
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	11	0.76
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	13	0.76
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	13	0.76
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	13	0.76
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	5	0.76
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	12	0.76
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	1	0.75
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	1	0.75
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	1	0.75
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	1	0.75
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	1	0.75
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	1	0.75
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	1	0.75
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	1	0.75
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	1	0.75
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	1	0.75
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	1	0.75
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	1	0.75
(1,2472)	2:B:686:LEU:HD12	2:B:610:LYS:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD11	2:B:610:LYS:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD13	2:B:610:LYS:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB3	8	0.75
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB3	8	0.75
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB2	8	0.75
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB3	8	0.75
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	8	0.75
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	7	0.75
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	9	0.75
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	2	0.75
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	13	0.75
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	8	0.75
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	8	0.75
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	8	0.75
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	12	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	15	0.74
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	10	0.74
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	14	0.74
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	14	0.74
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	14	0.74
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	5	0.74
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	14	0.74
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	4	0.74
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	3	0.74
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	3	0.74
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	3	0.74
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	3	0.73
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	3	0.73
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	3	0.73
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	11	0.73
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	11	0.73
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	11	0.73
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	14	0.73
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	14	0.73
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	14	0.73
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	7	0.73
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	6	0.73
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	1	0.73
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	3	0.73
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	6	0.73
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	7	0.73
(1,1308)	2:B:579:SER:HB2	1:A:39:SER:HG	7	0.73
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	11	0.73
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	11	0.73
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	11	0.73
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	7	0.72
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	7	0.72
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	7	0.72
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	7	0.72
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	7	0.72
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	7	0.72
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	7	0.72
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	7	0.72
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	7	0.72
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	13	0.72
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	13	0.72
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	13	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	6	0.72
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	6	0.72
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	6	0.72
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	6	0.72
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	6	0.72
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	6	0.72
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	6	0.72
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	6	0.72
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	6	0.72
(1,2152)	2:B:681:ASP:H	2:B:681:ASP:HB2	7	0.72
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	14	0.72
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	3	0.72
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	7	0.72
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	5	0.72
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	5	0.72
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	5	0.72
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	11	0.71
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	8	0.71
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	8	0.71
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	8	0.71
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	15	0.71
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	15	0.71
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	15	0.71
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	6	0.71
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	10	0.71
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	10	0.71
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	10	0.71
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	10	0.71
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	10	0.71
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	10	0.71
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	10	0.71
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	10	0.71
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	10	0.71
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	2	0.71
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	15	0.71
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	5	0.71
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	14	0.71
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	7	0.71
(1,1309)	2:B:579:SER:HB3	1:A:39:SER:HG	10	0.71
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD22	4	0.71
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD21	4	0.71
(1,1215)	2:B:681:ASP:HB3	2:B:677:LEU:HD23	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	14	0.71
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	11	0.71
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	11	0.71
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	11	0.71
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	8	0.7
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	14	0.7
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	9	0.7
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	9	0.7
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	11	0.7
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	11	0.7
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	11	0.7
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	11	0.7
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	11	0.7
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	11	0.7
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	11	0.7
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	11	0.7
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	11	0.7
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	4	0.7
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	4	0.7
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	7	0.7
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	6	0.7
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	9	0.7
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	15	0.7
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	2	0.7
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	8	0.7
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	9	0.7
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	12	0.7
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	13	0.7
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	6	0.7
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	6	0.7
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	6	0.7
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	7	0.69
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	7	0.69
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	7	0.69
(1,8)	2:B:568:PRO:HB3	2:B:569:PRO:HD3	7	0.69
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	10	0.69
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	10	0.69
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	10	0.69
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	11	0.69
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	11	0.69
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	11	0.69
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	11	0.69
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	11	0.69
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	11	0.69
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	11	0.69
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	11	0.69
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	5	0.69
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	5	0.69
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	5	0.69
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	1	0.69
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	1	0.69
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	9	0.69
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	15	0.69
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	12	0.69
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	13	0.69
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	4	0.69
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	11	0.69
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	10	0.69
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	11	0.69
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	2	0.68
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	2	0.68
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	2	0.68
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	2	0.68
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	2	0.68
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	2	0.68
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	2	0.68
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	2	0.68
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	2	0.68
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	12	0.68
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	12	0.68
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	12	0.68
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	12	0.68
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	12	0.68
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	12	0.68
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	12	0.68
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	12	0.68
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	12	0.68
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	2	0.68
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	3	0.68
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	10	0.68
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	5	0.68
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	13	0.68
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	4	0.68
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	4	0.68
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	15	0.68
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	8	0.68
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	8	0.68
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	8	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	5	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	5	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	5	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	11	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	11	0.68
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	11	0.68
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	5	0.67
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	5	0.67
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	5	0.67
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	8	0.67
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	8	0.67
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	8	0.67
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	12	0.67
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	12	0.67
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	12	0.67
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG2	1	0.67
(1,2675)	2:B:571:LEU:HD22	2:B:568:PRO:HG3	1	0.67
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG2	1	0.67
(1,2675)	2:B:571:LEU:HD21	2:B:568:PRO:HG3	1	0.67
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG2	1	0.67
(1,2675)	2:B:571:LEU:HD23	2:B:568:PRO:HG3	1	0.67
(1,2675)	2:B:571:LEU:HD22	2:B:569:PRO:HB3	1	0.67
(1,2675)	2:B:571:LEU:HD21	2:B:569:PRO:HB3	1	0.67
(1,2675)	2:B:571:LEU:HD23	2:B:569:PRO:HB3	1	0.67
(1,2675)	2:B:571:LEU:HD22	2:B:572:PRO:HG2	1	0.67
(1,2675)	2:B:571:LEU:HD21	2:B:572:PRO:HG2	1	0.67
(1,2675)	2:B:571:LEU:HD23	2:B:572:PRO:HG2	1	0.67
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	11	0.67
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	13	0.67
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	6	0.67
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	1	0.67
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	1	0.67
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	6	0.67
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	6	0.67
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	10	0.67
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG22	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG21	4	0.67
(1,1351)	1:A:37:TRP:HA	1:A:41:VAL:HG23	4	0.67
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	12	0.67
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	12	0.67
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	12	0.67
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	7	0.67
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	14	0.66
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	1	0.66
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	1	0.66
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	1	0.66
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	1	0.66
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	1	0.66
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	14	0.66
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	14	0.66
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	7	0.66
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	7	0.66
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	7	0.66
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	7	0.66
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	7	0.66
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	7	0.66
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	7	0.66
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	7	0.66
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	7	0.66
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	3	0.66
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	3	0.66
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	3	0.66
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	3	0.66
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	3	0.66
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	3	0.66
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	3	0.66
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	3	0.66
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	3	0.66
(1,2472)	2:B:686:LEU:HD12	2:B:610:LYS:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD11	2:B:610:LYS:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD13	2:B:610:LYS:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD12	2:B:688:LEU:HB3	1	0.66
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD11	2:B:688:LEU:HB3	1	0.66
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB2	1	0.66
(1,2472)	2:B:686:LEU:HD13	2:B:688:LEU:HB3	1	0.66
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	2	0.66
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	9	0.66
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	14	0.66
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	14	0.66
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	14	0.66
(1,1255)	2:B:672:LEU:HD12	2:B:592:GLU:HA	5	0.66
(1,1255)	2:B:672:LEU:HD11	2:B:592:GLU:HA	5	0.66
(1,1255)	2:B:672:LEU:HD13	2:B:592:GLU:HA	5	0.66
(1,487)	2:B:674:CYS:HB2	2:B:659:SER:HA	1	0.65
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	15	0.65
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	15	0.65
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	15	0.65
(1,1583)	2:B:596:THR:H	2:B:652:PHE:HZ	10	0.65
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	2	0.65
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	2	0.65
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	2	0.65
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	2	0.65
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	2	0.65
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	2	0.65
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	15	0.65
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	15	0.65
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	15	0.65
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD22	5	0.64
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD21	5	0.64
(1,562)	2:B:688:LEU:HD12	2:B:686:LEU:HD23	5	0.64
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD22	5	0.64
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD21	5	0.64
(1,562)	2:B:688:LEU:HD11	2:B:686:LEU:HD23	5	0.64
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD22	5	0.64
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD21	5	0.64
(1,562)	2:B:688:LEU:HD13	2:B:686:LEU:HD23	5	0.64
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	4	0.64
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	4	0.64
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	4	0.64
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	4	0.64
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	4	0.64
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	4	0.64
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	4	0.64
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	4	0.64
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	4	0.64
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	7	0.64
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	7	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	7	0.64
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	7	0.64
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	7	0.64
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	7	0.64
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	3	0.64
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	3	0.64
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	3	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	3	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	3	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	3	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	3	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	3	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	3	0.64
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	9	0.64
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	9	0.64
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	9	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	9	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	9	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	9	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	9	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	9	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	9	0.64
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	14	0.64
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	14	0.64
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	14	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	14	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	14	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	14	0.64
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	14	0.64
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	14	0.64
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	14	0.64
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD22	4	0.64
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD21	4	0.64
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD23	4	0.64
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	11	0.64
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	7	0.64
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	13	0.63
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	7	0.63
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	7	0.63
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	9	0.63
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	9	0.63
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	12	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	12	0.63
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	12	0.63
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	12	0.63
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	12	0.63
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	12	0.63
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	6	0.63
(1,2082)	2:B:670:PHE:H	2:B:575:PHE:HZ	14	0.63
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	5	0.63
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	4	0.63
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	12	0.63
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	3	0.63
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	4	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	3	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	3	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	3	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	5	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	5	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	5	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	11	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	11	0.63
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	11	0.63
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	1	0.62
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	3	0.62
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	14	0.62
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	14	0.62
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	14	0.62
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	4	0.62
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	13	0.62
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	12	0.62
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	12	0.62
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	15	0.62
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	15	0.62
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	15	0.62
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	15	0.62
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	15	0.62
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	15	0.62
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	15	0.62
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	15	0.62
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	15	0.62
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	9	0.62
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	9	0.62
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	9	0.62
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	9	0.62
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	9	0.62
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	14	0.62
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	14	0.62
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	14	0.62
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	14	0.62
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	14	0.62
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	14	0.62
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	5	0.62
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	5	0.62
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	5	0.62
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	5	0.62
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	5	0.62
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	5	0.62
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	5	0.62
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	5	0.62
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	5	0.62
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD22	15	0.62
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD21	15	0.62
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD23	15	0.62
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	12	0.62
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	12	0.62
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	12	0.62
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	13	0.62
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	13	0.62
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	13	0.62
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	11	0.62
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	14	0.62
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	8	0.62
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	9	0.61
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	9	0.61
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	9	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	9	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	9	0.61
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	9	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	9	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	9	0.61
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	9	0.61
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	10	0.61
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	10	0.61
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	10	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG22	15	0.61
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG21	15	0.61
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG23	15	0.61
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG22	15	0.61
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG21	15	0.61
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG23	15	0.61
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG22	15	0.61
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG21	15	0.61
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG23	15	0.61
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	14	0.61
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	14	0.61
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	11	0.61
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	11	0.61
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	11	0.61
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	1	0.61
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	1	0.61
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	1	0.61
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	1	0.61
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	1	0.61
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	1	0.61
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	13	0.61
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	13	0.61
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	13	0.61
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	13	0.61
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	13	0.61
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	13	0.61
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	13	0.61
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	13	0.61
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	13	0.61
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	12	0.61
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	7	0.61
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	7	0.61
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	7	0.61
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	8	0.61
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	13	0.61
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	9	0.61
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	9	0.61
(1,1468)	2:B:580:ILE:H	2:B:580:ILE:HG13	9	0.61
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG2	11	0.61
(1,1352)	1:A:47:SER:HA	1:A:48:GLN:HG3	11	0.61
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	3	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	6	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	6	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	15	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	15	0.61
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	15	0.61
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	13	0.61
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	9	0.61
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	9	0.61
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	9	0.61
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	2	0.61
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	2	0.61
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	2	0.61
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	3	0.6
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	3	0.6
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	3	0.6
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	3	0.6
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	3	0.6
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	3	0.6
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	3	0.6
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	3	0.6
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	3	0.6
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	8	0.6
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	8	0.6
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	8	0.6
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	8	0.6
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	8	0.6
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	8	0.6
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	11	0.6
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	11	0.6
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	11	0.6
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	11	0.6
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	11	0.6
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	11	0.6
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	15	0.6
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	15	0.6
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	15	0.6
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	15	0.6
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	15	0.6
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	15	0.6
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	1	0.6
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	1	0.6
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	15	0.6
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	5	0.6
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	5	0.6
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	10	0.6
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	10	0.6
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	10	0.6
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	8	0.6
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	8	0.6
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	8	0.6
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	15	0.59
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	11	0.59
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	11	0.59
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	11	0.59
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	10	0.59
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	10	0.59
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	10	0.59
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	10	0.59
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	10	0.59
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	10	0.59
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	10	0.59
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	10	0.59
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	10	0.59
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	5	0.59
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	5	0.59
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	5	0.59
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	5	0.59
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	5	0.59
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	5	0.59
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	1	0.59
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	1	0.59
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	1	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	1	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	1	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	1	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	1	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	1	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	1	0.59
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	2	0.59
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	2	0.59
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	2	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	2	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	2	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	2	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	2	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	2	0.59
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	6	0.59
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	6	0.59
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	6	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	6	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	6	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	6	0.59
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	6	0.59
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	6	0.59
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	6	0.59
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	1	0.59
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD22	5	0.59
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD21	5	0.59
(1,2138)	2:B:678:SER:H	2:B:677:LEU:HD23	5	0.59
(1,203)	2:B:609:LEU:HD12	2:B:609:LEU:HA	3	0.59
(1,203)	2:B:609:LEU:HD11	2:B:609:LEU:HA	3	0.59
(1,203)	2:B:609:LEU:HD13	2:B:609:LEU:HA	3	0.59
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	5	0.59
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	1	0.59
(1,1605)	2:B:598:ASP:H	2:B:597:GLU:HG2	13	0.59
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	12	0.59
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	12	0.58
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	1	0.58
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	5	0.58
(1,512)	2:B:679:VAL:HG12	2:B:619:ILE:HD12	4	0.58
(1,512)	2:B:679:VAL:HG12	2:B:619:ILE:HD11	4	0.58
(1,512)	2:B:679:VAL:HG12	2:B:619:ILE:HD13	4	0.58
(1,512)	2:B:679:VAL:HG11	2:B:619:ILE:HD12	4	0.58
(1,512)	2:B:679:VAL:HG11	2:B:619:ILE:HD11	4	0.58
(1,512)	2:B:679:VAL:HG11	2:B:619:ILE:HD13	4	0.58
(1,512)	2:B:679:VAL:HG13	2:B:619:ILE:HD12	4	0.58
(1,512)	2:B:679:VAL:HG13	2:B:619:ILE:HD11	4	0.58
(1,512)	2:B:679:VAL:HG13	2:B:619:ILE:HD13	4	0.58
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	1	0.58
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	1	0.58
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	1	0.58
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	4	0.58
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	4	0.58
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	7	0.58
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	7	0.58
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	7	0.58
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	7	0.58
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	7	0.58
(1,2530)	2:B:682:VAL:HG22	2:B:613:SER:HB3	9	0.58
(1,2530)	2:B:682:VAL:HG21	2:B:613:SER:HB3	9	0.58
(1,2530)	2:B:682:VAL:HG23	2:B:613:SER:HB3	9	0.58
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG12	9	0.58
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG11	9	0.58
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG13	9	0.58
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	2	0.58
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	2	0.58
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	2	0.58
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	2	0.58
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	2	0.58
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	2	0.58
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	6	0.58
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	6	0.58
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	6	0.58
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	6	0.58
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	6	0.58
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	6	0.58
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	10	0.58
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	10	0.58
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	10	0.58
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	10	0.58
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	10	0.58
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	10	0.58
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	13	0.58
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	13	0.58
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	13	0.58
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	13	0.58
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	13	0.58
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	13	0.58
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	15	0.58
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	5	0.58
(1,1774)	2:B:621:ASP:H	2:B:620:GLU:HB2	11	0.58
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	7	0.58
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	1	0.58
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	1	0.58
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	15	0.58
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	3	0.58
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	11	0.58
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	12	0.58
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	4	0.57
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	4	0.57
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	4	0.57
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	7	0.57
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	2	0.57
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	2	0.57
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	2	0.57
(1,394)	2:B:646:LEU:HD22	2:B:646:LEU:HA	3	0.57
(1,394)	2:B:646:LEU:HD21	2:B:646:LEU:HA	3	0.57
(1,394)	2:B:646:LEU:HD23	2:B:646:LEU:HA	3	0.57
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	4	0.57
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	4	0.57
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	4	0.57
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	4	0.57
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	4	0.57
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	4	0.57
(1,2431)	2:B:646:LEU:HD12	1:A:40:LEU:HA	4	0.57
(1,2431)	2:B:646:LEU:HD11	1:A:40:LEU:HA	4	0.57
(1,2431)	2:B:646:LEU:HD13	1:A:40:LEU:HA	4	0.57
(1,2431)	2:B:646:LEU:HD12	2:B:625:PRO:HA	4	0.57
(1,2431)	2:B:646:LEU:HD11	2:B:625:PRO:HA	4	0.57
(1,2431)	2:B:646:LEU:HD13	2:B:625:PRO:HA	4	0.57
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	9	0.57
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	11	0.57
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	10	0.57
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	10	0.57
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	10	0.57
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	14	0.57
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	14	0.57
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	14	0.57
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	15	0.57
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	15	0.57
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	15	0.57
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	1	0.57
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	14	0.57
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	14	0.57
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	14	0.57
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG22	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG21	10	0.57
(1,1067)	2:B:582:GLN:HG2	2:B:580:ILE:HG23	10	0.57
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	1	0.56
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	14	0.56
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	9	0.56
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	11	0.56
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	9	0.56
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	13	0.56
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	13	0.56
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	13	0.56
(1,1251)	2:B:594:LEU:HD12	2:B:658:TRP:HZ2	10	0.56
(1,1251)	2:B:594:LEU:HD11	2:B:658:TRP:HZ2	10	0.56
(1,1251)	2:B:594:LEU:HD13	2:B:658:TRP:HZ2	10	0.56
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	13	0.56
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD12	14	0.55
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD11	14	0.55
(1,976)	2:B:574:TYR:HB2	2:B:581:ILE:HD13	14	0.55
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	7	0.55
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	10	0.55
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	11	0.55
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	11	0.55
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	11	0.55
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	11	0.55
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	11	0.55
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	11	0.55
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	11	0.55
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	11	0.55
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	11	0.55
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	11	0.55
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	11	0.55
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	1	0.55
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	1	0.55
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	1	0.55
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	1	0.55
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	1	0.55
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	1	0.55
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	1	0.55
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	1	0.55
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	1	0.55
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	9	0.55
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	4	0.55
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	4	0.55
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	3	0.55
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	9	0.55
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	2	0.55
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	11	0.54
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	13	0.54
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	13	0.54
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	13	0.54
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	14	0.54
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	6	0.54
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	6	0.54
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	6	0.54
(1,2530)	2:B:682:VAL:HG22	2:B:613:SER:HB3	14	0.54
(1,2530)	2:B:682:VAL:HG21	2:B:613:SER:HB3	14	0.54
(1,2530)	2:B:682:VAL:HG23	2:B:613:SER:HB3	14	0.54
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG12	14	0.54
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG11	14	0.54
(1,2530)	2:B:642:SER:HB3	2:B:629:VAL:HG13	14	0.54
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	15	0.54
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	15	0.54
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	15	0.54
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	15	0.54
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	15	0.54
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	15	0.54
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	15	0.54
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	15	0.54
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	15	0.54
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	1	0.54
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	12	0.54
(1,1560)	2:B:592:GLU:H	2:B:672:LEU:HD12	9	0.54
(1,1560)	2:B:592:GLU:H	2:B:672:LEU:HD11	9	0.54
(1,1560)	2:B:592:GLU:H	2:B:672:LEU:HD13	9	0.54
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	4	0.54
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	2	0.54
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	2	0.54
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	2	0.54
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	13	0.54
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	13	0.54
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	13	0.54
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	7	0.54
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	12	0.53
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	3	0.53
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	3	0.53
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	12	0.53
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	12	0.53
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	12	0.53
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	6	0.53
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	6	0.53
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	12	0.53
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	12	0.53
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	12	0.53
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	5	0.53
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	10	0.53
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	7	0.53
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	2	0.53
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	3	0.53
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	6	0.53
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	9	0.53
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	14	0.53
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	2	0.53
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	2	0.53
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	2	0.53
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	3	0.53
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	8	0.52
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	13	0.52
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	8	0.52
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	8	0.52
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	8	0.52
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	8	0.52
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	8	0.52
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	8	0.52
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	8	0.52
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	8	0.52
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	8	0.52
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	2	0.52
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	2	0.52
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	2	0.52
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	8	0.52
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	3	0.52
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	14	0.52
(1,1543)	2:B:590:LYS:H	2:B:590:LYS:HB3	15	0.52
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	7	0.52
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	7	0.52
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	1	0.52
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	7	0.52
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	8	0.52
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	10	0.52
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	6	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	6	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	6	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	11	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	11	0.51
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	11	0.51
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	2	0.51
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	3	0.51
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	4	0.51
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	11	0.51
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG22	5	0.51
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG21	5	0.51
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG23	5	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG22	5	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG21	5	0.51
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG23	5	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG22	5	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG21	5	0.51
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG23	5	0.51
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	4	0.51
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	4	0.51
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	4	0.51
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	4	0.51
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	1	0.51
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	1	0.51
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	1	0.51
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	1	0.51
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	1	0.51
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	1	0.51
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	1	0.51
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	1	0.51
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	1	0.51
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	14	0.51
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	15	0.51
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	4	0.51
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	15	0.51
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	6	0.51
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	6	0.51
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	8	0.51
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	8	0.51
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	8	0.51
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	11	0.51
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	6	0.51
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	12	0.51
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	14	0.51
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	3	0.51
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	11	0.51
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	5	0.51
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	7	0.5
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG22	2	0.5
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG21	2	0.5
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG23	2	0.5
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	8	0.5
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	11	0.5
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	13	0.5
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	13	0.5
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	13	0.5
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	13	0.5
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	13	0.5
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	13	0.5
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	13	0.5
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	13	0.5
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	13	0.5
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	6	0.5
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	4	0.5
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	6	0.5
(1,1604)	2:B:598:ASP:H	2:B:598:ASP:HB2	10	0.5
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	4	0.5
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	4	0.5
(1,1454)	2:B:579:SER:H	2:B:579:SER:HB2	15	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	1	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	1	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	1	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	3	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	3	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	3	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	8	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	8	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	14	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	14	0.5
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	14	0.5
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	8	0.5
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	9	0.5
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	1	0.5
(1,1109)	2:B:672:LEU:HG	2:B:673:PRO:HD3	6	0.5
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD12	4	0.49
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD11	4	0.49
(1,775)	2:B:612:ASP:HB2	1:A:44:LEU:HD13	4	0.49
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	10	0.49
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG22	4	0.49
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG21	4	0.49
(1,501)	2:B:677:LEU:HD12	2:B:630:ILE:HG23	4	0.49
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG22	4	0.49
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG21	4	0.49
(1,501)	2:B:677:LEU:HD11	2:B:630:ILE:HG23	4	0.49
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG22	4	0.49
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG21	4	0.49
(1,501)	2:B:677:LEU:HD13	2:B:630:ILE:HG23	4	0.49
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	15	0.49
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	15	0.49
(1,2069)	2:B:668:GLN:H	2:B:667:SER:HB3	12	0.49
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG2	1	0.49
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG3	1	0.49
(1,1454)	2:B:579:SER:H	2:B:579:SER:HB2	13	0.49
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	4	0.49
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	10	0.49
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	11	0.49
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	5	0.49
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	2	0.49
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	15	0.48
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	15	0.48
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	15	0.48
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	6	0.48
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	15	0.48
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD22	9	0.48
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD21	9	0.48
(1,637)	2:B:658:TRP:HB2	2:B:672:LEU:HD23	9	0.48
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	1	0.48
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	1	0.48
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HG2	8	0.48
(1,2607)	2:B:659:SER:HA	2:B:673:PRO:HB2	8	0.48
(1,2607)	2:B:659:SER:HA	1:A:40:LEU:HB2	8	0.48
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	12	0.48
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	12	0.48
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	12	0.48
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	12	0.48
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	12	0.48
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	12	0.48
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	12	0.48
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	12	0.48
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	12	0.48
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	11	0.48
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	11	0.48
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	11	0.48
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	10	0.48
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	13	0.48
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	9	0.48
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	2	0.48
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	7	0.48
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	9	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	3	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	3	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	3	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	14	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	14	0.48
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	14	0.48
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	8	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	6	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	6	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	6	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	9	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	9	0.48
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	9	0.48
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	2	0.48
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	5	0.48
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	13	0.48
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	13	0.48
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	7	0.47
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	7	0.47
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	13	0.47
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	13	0.47
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	13	0.47
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	13	0.47
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	13	0.47
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	13	0.47
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	5	0.47
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	5	0.47
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	5	0.47
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	2	0.47
(1,1988)	2:B:656:GLN:H	2:B:656:GLN:HB3	6	0.47
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	5	0.47
(1,1773)	2:B:621:ASP:H	2:B:621:ASP:HB3	7	0.47
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	12	0.47
(1,1250)	2:B:619:ILE:HG12	2:B:618:ARG:H	4	0.47
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	10	0.47
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	2	0.47
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	11	0.47
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	12	0.47
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD22	9	0.47
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD21	9	0.47
(1,1056)	2:B:666:THR:HG21	2:B:672:LEU:HD23	9	0.47
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD22	9	0.47
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD21	9	0.47
(1,1056)	2:B:666:THR:HG22	2:B:672:LEU:HD23	9	0.47
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD22	9	0.47
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD21	9	0.47
(1,1056)	2:B:666:THR:HG23	2:B:672:LEU:HD23	9	0.47
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	4	0.46
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	4	0.46
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	4	0.46
(1,638)	2:B:658:TRP:HB2	2:B:593:ASP:HA	10	0.46
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	13	0.46
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	2	0.46
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	2	0.46
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	2	0.46
(1,2422)	2:B:643:VAL:HG12	1:A:48:GLN:HE21	9	0.46
(1,2422)	2:B:643:VAL:HG11	1:A:48:GLN:HE21	9	0.46
(1,2422)	2:B:643:VAL:HG13	1:A:48:GLN:HE21	9	0.46
(1,2422)	2:B:643:VAL:HG12	2:B:640:GLN:HE22	9	0.46
(1,2422)	2:B:643:VAL:HG11	2:B:640:GLN:HE22	9	0.46
(1,2422)	2:B:643:VAL:HG13	2:B:640:GLN:HE22	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE1	9	0.46
(1,2422)	2:B:682:VAL:HG12	2:B:652:PHE:HE2	9	0.46
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE1	9	0.46
(1,2422)	2:B:682:VAL:HG11	2:B:652:PHE:HE2	9	0.46
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE1	9	0.46
(1,2422)	2:B:682:VAL:HG13	2:B:652:PHE:HE2	9	0.46
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	11	0.46
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	11	0.46
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	11	0.46
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	2	0.46
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	2	0.46
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	2	0.46
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	9	0.46
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	9	0.46
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	9	0.46
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	15	0.46
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	15	0.46
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	15	0.46
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	10	0.46
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	13	0.46
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	8	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	2	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	2	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	2	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	5	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	5	0.46
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	5	0.46
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	4	0.46
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	5	0.46
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	5	0.46
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	5	0.46
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	5	0.46
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	5	0.46
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	5	0.46
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	1	0.46
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	5	0.46
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	10	0.46
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	11	0.46
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	15	0.46
(1,1113)	2:B:674:CYS:HA	2:B:663:PRO:HB2	6	0.46
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	10	0.45
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	10	0.45
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	6	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	4	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	4	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	4	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	4	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	4	0.45
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	4	0.45
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	7	0.45
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	7	0.45
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	7	0.45
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	7	0.45
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	7	0.45
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	7	0.45
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	7	0.45
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	7	0.45
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	7	0.45
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	15	0.45
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	15	0.45
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	15	0.45
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	11	0.45
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	15	0.45
(1,2069)	2:B:668:GLN:H	2:B:667:SER:HB3	4	0.45
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	2	0.45
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	7	0.45
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	8	0.45
(1,2065)	2:B:667:SER:H	2:B:667:SER:HB3	10	0.45
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG2	7	0.45
(1,2045)	2:B:664:GLU:H	2:B:664:GLU:HG3	7	0.45
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	11	0.45
(1,1773)	2:B:621:ASP:H	2:B:621:ASP:HB3	13	0.45
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	13	0.45
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	1	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	2	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	2	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	2	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	12	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	12	0.45
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	12	0.45
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	11	0.45
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD22	5	0.45
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD21	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD23	5	0.45
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	4	0.45
(1,1168)	2:B:686:LEU:HD12	2:B:609:LEU:HB2	8	0.45
(1,1168)	2:B:686:LEU:HD11	2:B:609:LEU:HB2	8	0.45
(1,1168)	2:B:686:LEU:HD13	2:B:609:LEU:HB2	8	0.45
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	12	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	1	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	13	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	13	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	13	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	13	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	13	0.44
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	13	0.44
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	5	0.44
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	5	0.44
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	5	0.44
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	5	0.44
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	5	0.44
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	5	0.44
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	5	0.44
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	5	0.44
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	5	0.44
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	3	0.44
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	3	0.44
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	3	0.44
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	15	0.44
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	10	0.44
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	5	0.44
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	14	0.44
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	3	0.44
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	12	0.44
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	5	0.44
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	5	0.44
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	5	0.44
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	12	0.44
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	15	0.44
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	4	0.44
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	4	0.44
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	4	0.44
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	3	0.43
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	3	0.43
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	3	0.43
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	10	0.43
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	10	0.43
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	10	0.43
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	10	0.43
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	10	0.43
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	10	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	7	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	7	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	7	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	7	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	7	0.43
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	7	0.43
(1,2357)	2:B:616:VAL:HG12	1:A:44:LEU:HG	11	0.43
(1,2357)	2:B:616:VAL:HG11	1:A:44:LEU:HG	11	0.43
(1,2357)	2:B:616:VAL:HG13	1:A:44:LEU:HG	11	0.43
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HG12	11	0.43
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HG12	11	0.43
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HG12	11	0.43
(1,2357)	2:B:616:VAL:HG12	2:B:630:ILE:HB	11	0.43
(1,2357)	2:B:616:VAL:HG11	2:B:630:ILE:HB	11	0.43
(1,2357)	2:B:616:VAL:HG13	2:B:630:ILE:HB	11	0.43
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	10	0.43
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	10	0.43
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	10	0.43
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	1	0.43
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	7	0.43
(1,2069)	2:B:668:GLN:H	2:B:667:SER:HB3	15	0.43
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	1	0.43
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	12	0.43
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	15	0.43
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	10	0.43
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	10	0.43
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	10	0.43
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	10	0.43
(1,103)	2:B:672:LEU:HD12	2:B:672:LEU:HA	9	0.43
(1,103)	2:B:672:LEU:HD11	2:B:672:LEU:HA	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	2:B:672:LEU:HD13	2:B:672:LEU:HA	9	0.43
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	7	0.42
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	13	0.42
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	6	0.42
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	6	0.42
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	6	0.42
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	8	0.42
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	8	0.42
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	8	0.42
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	10	0.42
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	10	0.42
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	10	0.42
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	9	0.42
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	9	0.42
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	1	0.42
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	1	0.42
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	1	0.42
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	1	0.42
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	1	0.42
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	1	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	2	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	2	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	2	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	2	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	2	0.42
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	2	0.42
(1,22)	2:B:571:LEU:HD22	2:B:571:LEU:HA	1	0.42
(1,22)	2:B:571:LEU:HD21	2:B:571:LEU:HA	1	0.42
(1,22)	2:B:571:LEU:HD23	2:B:571:LEU:HA	1	0.42
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	1	0.42
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	1	0.42
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	1	0.42
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	7	0.42
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	1	0.42
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	1	0.42
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	1	0.42
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	1	0.42
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	1	0.42
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	1	0.42
(1,1364)	1:A:47:SER:HA	1:A:48:GLN:HB3	10	0.42
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	7	0.42
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	7	0.42
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	1	0.42
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	14	0.42
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	5	0.41
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	7	0.41
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	7	0.41
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	7	0.41
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	6	0.41
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	13	0.41
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	13	0.41
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	13	0.41
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	15	0.41
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	2	0.41
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	2	0.41
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	2	0.41
(1,204)	2:B:609:LEU:HD12	2:B:688:LEU:HA	3	0.41
(1,204)	2:B:609:LEU:HD11	2:B:688:LEU:HA	3	0.41
(1,204)	2:B:609:LEU:HD13	2:B:688:LEU:HA	3	0.41
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	7	0.41
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	6	0.41
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	9	0.41
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	8	0.41
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	10	0.41
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	11	0.41
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	1	0.41
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	6	0.41
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	7	0.41
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	9	0.41
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	9	0.41
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	9	0.41
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	3	0.41
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	8	0.41
(1,896)	2:B:630:ILE:HD12	2:B:651:PHE:HE1	5	0.4
(1,896)	2:B:630:ILE:HD12	2:B:651:PHE:HE2	5	0.4
(1,896)	2:B:630:ILE:HD11	2:B:651:PHE:HE1	5	0.4
(1,896)	2:B:630:ILE:HD11	2:B:651:PHE:HE2	5	0.4
(1,896)	2:B:630:ILE:HD13	2:B:651:PHE:HE1	5	0.4
(1,896)	2:B:630:ILE:HD13	2:B:651:PHE:HE2	5	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	7	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	7	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	7	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	14	0.4
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	14	0.4
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	9	0.4
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	9	0.4
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	9	0.4
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	8	0.4
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	8	0.4
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	8	0.4
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	8	0.4
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	8	0.4
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	8	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	9	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	14	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	14	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	14	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	14	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	14	0.4
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	14	0.4
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	4	0.4
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	6	0.4
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	13	0.4
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	10	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	4	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	4	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	4	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	11	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	11	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	11	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	15	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	15	0.4
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	15	0.4
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	13	0.4
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	13	0.4
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	1	0.4
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	14	0.4
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	1	0.4
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	5	0.4
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	6	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	11	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	11	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	11	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD12	12	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD11	12	0.4
(1,1353)	1:A:44:LEU:HA	1:A:44:LEU:HD13	12	0.4
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	14	0.4
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	5	0.4
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	6	0.4
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	12	0.4
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	6	0.39
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	5	0.39
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	5	0.39
(1,553)	2:B:686:LEU:HD12	2:B:686:LEU:HA	8	0.39
(1,553)	2:B:686:LEU:HD11	2:B:686:LEU:HA	8	0.39
(1,553)	2:B:686:LEU:HD13	2:B:686:LEU:HA	8	0.39
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	10	0.39
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	10	0.39
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	10	0.39
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	4	0.39
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	10	0.39
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	13	0.39
(1,2352)	2:B:653:VAL:HG12	2:B:681:ASP:HB2	7	0.39
(1,2352)	2:B:653:VAL:HG11	2:B:681:ASP:HB2	7	0.39
(1,2352)	2:B:653:VAL:HG13	2:B:681:ASP:HB2	7	0.39
(1,2352)	2:B:653:VAL:HG12	2:B:683:CYS:HB3	7	0.39
(1,2352)	2:B:653:VAL:HG11	2:B:683:CYS:HB3	7	0.39
(1,2352)	2:B:653:VAL:HG13	2:B:683:CYS:HB3	7	0.39
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	3	0.39
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	3	0.39
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	3	0.39
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	3	0.39
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	3	0.39
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	3	0.39
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	3	0.39
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	3	0.39
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	3	0.39
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	7	0.39
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	5	0.39
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	2:B:620:GLU:H	2:B:620:GLU:HB3	5	0.39
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	3	0.39
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	1	0.39
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	14	0.39
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	1	0.39
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	1	0.39
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	1	0.39
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	14	0.39
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	11	0.38
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	11	0.38
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	11	0.38
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	10	0.38
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG2	14	0.38
(1,2674)	2:B:571:LEU:HD12	2:B:568:PRO:HG3	14	0.38
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG2	14	0.38
(1,2674)	2:B:571:LEU:HD11	2:B:568:PRO:HG3	14	0.38
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG2	14	0.38
(1,2674)	2:B:571:LEU:HD13	2:B:568:PRO:HG3	14	0.38
(1,2674)	2:B:571:LEU:HD12	2:B:569:PRO:HB3	14	0.38
(1,2674)	2:B:571:LEU:HD11	2:B:569:PRO:HB3	14	0.38
(1,2674)	2:B:571:LEU:HD13	2:B:569:PRO:HB3	14	0.38
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	11	0.38
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	12	0.38
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	12	0.38
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	12	0.38
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	12	0.38
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	12	0.38
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	12	0.38
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	4	0.38
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	4	0.38
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	4	0.38
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	8	0.38
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	8	0.38
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	8	0.38
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	8	0.38
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	8	0.38
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	8	0.38
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	8	0.38
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	8	0.38
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	8	0.38
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	14	0.38
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	14	0.38
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	14	0.38
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	14	0.38
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	14	0.38
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	14	0.38
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	14	0.38
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	14	0.38
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	6	0.38
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	6	0.38
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	6	0.38
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	15	0.38
(1,2108)	2:B:674:CYS:H	2:B:673:PRO:HB2	2	0.38
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	12	0.38
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	14	0.38
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	13	0.38
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	13	0.38
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	14	0.38
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	7	0.38
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	3	0.37
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	3	0.37
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	3	0.37
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	1	0.37
(1,524)	2:B:653:VAL:HG12	2:B:681:ASP:HB2	7	0.37
(1,524)	2:B:653:VAL:HG11	2:B:681:ASP:HB2	7	0.37
(1,524)	2:B:653:VAL:HG13	2:B:681:ASP:HB2	7	0.37
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	1	0.37
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	1	0.37
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	1	0.37
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	5	0.37
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	5	0.37
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	5	0.37
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	6	0.37
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	6	0.37
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	6	0.37
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	6	0.37
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	8	0.37
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	8	0.37
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	8	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	8	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	8	0.37
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	8	0.37
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	8	0.37
(1,259)	2:B:617:GLU:HG3	2:B:617:GLU:HA	15	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	3	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	3	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	3	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	3	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	3	0.37
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	3	0.37
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	7	0.37
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	13	0.37
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	5	0.37
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	12	0.37
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	12	0.37
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	3	0.37
(1,553)	2:B:686:LEU:HD12	2:B:686:LEU:HA	1	0.36
(1,553)	2:B:686:LEU:HD11	2:B:686:LEU:HA	1	0.36
(1,553)	2:B:686:LEU:HD13	2:B:686:LEU:HA	1	0.36
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	5	0.36
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	7	0.36
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	13	0.36
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	13	0.36
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	15	0.36
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	15	0.36
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	15	0.36
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	14	0.36
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	14	0.36
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	14	0.36
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	14	0.36
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	14	0.36
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	14	0.36
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD1	9	0.36
(1,2523)	2:B:611:ILE:HD12	1:A:43:PHE:HD2	9	0.36
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD1	9	0.36
(1,2523)	2:B:611:ILE:HD11	1:A:43:PHE:HD2	9	0.36
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD1	9	0.36
(1,2523)	2:B:611:ILE:HD13	1:A:43:PHE:HD2	9	0.36
(1,2523)	2:B:611:ILE:HD12	2:B:584:ALA:H	9	0.36
(1,2523)	2:B:611:ILE:HD11	2:B:584:ALA:H	9	0.36
(1,2523)	2:B:611:ILE:HD13	2:B:584:ALA:H	9	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	1	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	1	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	1	0.36
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	1	0.36
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	1	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	1	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	1	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	1	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	9	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	9	0.36
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	9	0.36
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	9	0.36
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	9	0.36
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	9	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	9	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	9	0.36
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	9	0.36
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	14	0.36
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	12	0.36
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	10	0.36
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	15	0.36
(1,1902)	2:B:640:GLN:H	2:B:640:GLN:HG3	4	0.36
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	2	0.36
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	6	0.36
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	8	0.36
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	10	0.36
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	15	0.36
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	11	0.36
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	15	0.36
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	4	0.36
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	8	0.36
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	2	0.35
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	2	0.35
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	2	0.35
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	4	0.35
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	4	0.35
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	4	0.35
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG22	14	0.35
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG21	14	0.35
(1,423)	2:B:654:PHE:HB2	2:B:682:VAL:HG23	14	0.35
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	5	0.35
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	5	0.35
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	5	0.35
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	15	0.35
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	15	0.35
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	11	0.35
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	11	0.35
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	11	0.35
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	11	0.35
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	11	0.35
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	11	0.35
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	11	0.35
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	6	0.35
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	6	0.35
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	6	0.35
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	6	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	8	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	11	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	11	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	11	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	11	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	11	0.35
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	11	0.35
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	5	0.35
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	15	0.35
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	3	0.35
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	3	0.35
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	4	0.35
(1,1902)	2:B:640:GLN:H	2:B:640:GLN:HG3	12	0.35
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	11	0.35
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	12	0.35
(1,1425)	2:B:571:LEU:H	2:B:571:LEU:HB2	3	0.35
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	8	0.35
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	9	0.35
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG22	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG21	8	0.35
(1,1256)	2:B:592:GLU:HA	2:B:591:VAL:HG23	8	0.35
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	11	0.35
(1,116)	2:B:578:GLY:HA3	2:B:590:LYS:HD3	14	0.35
(1,1117)	2:B:589:LYS:HB2	2:B:589:LYS:HE2	9	0.35
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	1	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	1	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	1	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	6	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	6	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	6	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	8	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	8	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	8	0.34
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	15	0.34
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	11	0.34
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	11	0.34
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	11	0.34
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	12	0.34
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	9	0.34
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	12	0.34
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	7	0.34
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	7	0.34
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	7	0.34
(1,2209)	2:B:576:MET:HB2	1:A:39:SER:HG	3	0.34
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	10	0.34
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	13	0.34
(1,2070)	2:B:668:GLN:H	2:B:668:GLN:HG2	6	0.34
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	1	0.34
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	1	0.34
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	8	0.34
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	3	0.34
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	11	0.34
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	4	0.34
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	10	0.34
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	14	0.34
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	14	0.34
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	14	0.34
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	15	0.34
(1,1424)	2:B:571:LEU:H	2:B:570:THR:HA	4	0.34
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	3	0.34
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	3	0.34
(1,1389)	1:A:37:TRP:HB3	1:A:37:TRP:HE3	7	0.34
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	14	0.33
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	14	0.33
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	14	0.33
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	5	0.33
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	8	0.33
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	8	0.33
(1,2134)	2:B:678:SER:H	2:B:681:ASP:HB2	7	0.33
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	8	0.33
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	13	0.33
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	4	0.33
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	11	0.33
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	14	0.33
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	9	0.33
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	2	0.33
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	2	0.33
(1,1607)	2:B:598:ASP:H	2:B:595:LYS:HB3	10	0.33
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	2	0.33
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	7	0.33
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	7	0.33
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	15	0.32
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	15	0.32
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	15	0.32
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	14	0.32
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	15	0.32
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	15	0.32
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	15	0.32
(1,420)	2:B:654:PHE:HB2	2:B:682:VAL:HB	3	0.32
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	1	0.32
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	9	0.32
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	14	0.32
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	6	0.32
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	6	0.32
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	6	0.32
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	6	0.32
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	12	0.32
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	12	0.32
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	12	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	10	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	10	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	10	0.32
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	10	0.32
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	10	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	15	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	15	0.32
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	15	0.32
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	15	0.32
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	15	0.32
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	15	0.32
(1,2277)	2:B:639:ALA:HB2	1:A:48:GLN:HB3	6	0.32
(1,2277)	2:B:639:ALA:HB1	1:A:48:GLN:HB3	6	0.32
(1,2277)	2:B:639:ALA:HB3	1:A:48:GLN:HB3	6	0.32
(1,2222)	2:B:686:LEU:HD22	1:A:38:HIS:HB2	7	0.32
(1,2222)	2:B:686:LEU:HD21	1:A:38:HIS:HB2	7	0.32
(1,2222)	2:B:686:LEU:HD23	1:A:38:HIS:HB2	7	0.32
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	6	0.32
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	2	0.32
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	8	0.32
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	8	0.32
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	8	0.32
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	11	0.32
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	13	0.32
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	7	0.32
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	14	0.32
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD22	4	0.32
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD21	4	0.32
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD23	4	0.32
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD22	4	0.32
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD21	4	0.32
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD23	4	0.32
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	12	0.32
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	3	0.32
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	3	0.32
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	14	0.32
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	14	0.32
(1,101)	2:B:672:LEU:HD12	2:B:591:VAL:HB	5	0.32
(1,101)	2:B:672:LEU:HD11	2:B:591:VAL:HB	5	0.32
(1,101)	2:B:672:LEU:HD13	2:B:591:VAL:HB	5	0.32
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	12	0.31
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	14	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	9	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	9	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	10	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	10	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	10	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	13	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	13	0.31
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	13	0.31
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	8	0.31
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	8	0.31
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	8	0.31
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	8	0.31
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	10	0.31
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	13	0.31
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	15	0.31
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	11	0.31
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	11	0.31
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	11	0.31
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	11	0.31
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	11	0.31
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	11	0.31
(1,2451)	2:B:674:CYS:HB2	1:A:40:LEU:HB2	2	0.31
(1,2451)	2:B:674:CYS:HB2	2:B:673:PRO:HG2	2	0.31
(1,2451)	2:B:674:CYS:HB2	2:B:673:PRO:HB2	2	0.31
(1,2385)	2:B:656:GLN:HG2	2:B:682:VAL:HA	12	0.31
(1,2385)	2:B:656:GLN:HG2	2:B:680:GLY:HA2	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	12	0.31
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	12	0.31
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	12	0.31
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	12	0.31
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	12	0.31
(1,2108)	2:B:674:CYS:H	2:B:673:PRO:HB2	13	0.31
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	9	0.31
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	15	0.31
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	4	0.31
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	1	0.31
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	5	0.31
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	2	0.31
(1,1730)	2:B:617:GLU:H	2:B:617:GLU:HB3	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	10	0.31
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	12	0.31
(1,1649)	2:B:602:SER:H	2:B:602:SER:HB2	14	0.31
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	15	0.31
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	6	0.31
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	6	0.31
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	1	0.31
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	1	0.31
(1,107)	2:B:672:LEU:HD22	2:B:672:LEU:HA	8	0.31
(1,107)	2:B:672:LEU:HD21	2:B:672:LEU:HA	8	0.31
(1,107)	2:B:672:LEU:HD23	2:B:672:LEU:HA	8	0.31
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	15	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	2	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	2	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	2	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	4	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	4	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	4	0.3
(1,521)	2:B:679:VAL:HG22	2:B:680:GLY:HA2	4	0.3
(1,521)	2:B:679:VAL:HG21	2:B:680:GLY:HA2	4	0.3
(1,521)	2:B:679:VAL:HG23	2:B:680:GLY:HA2	4	0.3
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	3	0.3
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	4	0.3
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	7	0.3
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	7	0.3
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	7	0.3
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	9	0.3
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	9	0.3
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	9	0.3
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	9	0.3
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	9	0.3
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	9	0.3
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB2	15	0.3
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB3	15	0.3
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	11	0.3
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	5	0.3
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	5	0.3
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	5	0.3
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	3	0.3
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	15	0.3
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	7	0.3
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	7	0.3
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	11	0.3
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	14	0.3
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	5	0.29
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	5	0.29
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	5	0.29
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG21	12	0.29
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG22	12	0.29
(1,801)	2:B:680:GLY:HA3	2:B:615:THR:HG23	12	0.29
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	9	0.29
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	13	0.29
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	13	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	2	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	2	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	2	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	2	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	2	0.29
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	2	0.29
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	3	0.29
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	1	0.29
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	1	0.29
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	1	0.29
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	11	0.29
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	7	0.29
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG22	9	0.29
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG21	9	0.29
(1,1709)	2:B:614:SER:H	2:B:682:VAL:HG23	9	0.29
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	13	0.29
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	13	0.29
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	13	0.29
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	9	0.29
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	9	0.29
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	9	0.29
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	3	0.28
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	13	0.28
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	9	0.28
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	9	0.28
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	9	0.28
(1,515)	2:B:679:VAL:HG12	2:B:618:ARG:HA	14	0.28
(1,515)	2:B:679:VAL:HG11	2:B:618:ARG:HA	14	0.28
(1,515)	2:B:679:VAL:HG13	2:B:618:ARG:HA	14	0.28
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	3	0.28
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	3	0.28
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	3	0.28
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	3	0.28
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	3	0.28
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	3	0.28
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	5	0.28
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	5	0.28
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	5	0.28
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	5	0.28
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	5	0.28
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	5	0.28
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	5	0.28
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	5	0.28
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	5	0.28
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	5	0.28
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	5	0.28
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	5	0.28
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	10	0.28
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	10	0.28
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	10	0.28
(1,2200)	2:B:689:LYS:H	2:B:609:LEU:HD12	15	0.28
(1,2200)	2:B:689:LYS:H	2:B:609:LEU:HD11	15	0.28
(1,2200)	2:B:689:LYS:H	2:B:609:LEU:HD13	15	0.28
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	7	0.28
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	9	0.28
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	9	0.28
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	9	0.28
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	1	0.28
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	3	0.28
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	11	0.28
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	7	0.28
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	5	0.28
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	12	0.28
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	1	0.28
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	9	0.28
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	15	0.28
(1,1753)	2:B:619:ILE:H	2:B:619:ILE:HG12	4	0.28
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	9	0.28
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	9	0.28
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	9	0.28
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	15	0.28
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	9	0.28
(1,1424)	2:B:571:LEU:H	2:B:570:THR:HA	11	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD12	13	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD11	13	0.28
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD13	13	0.28
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	1	0.27
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	13	0.27
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	13	0.27
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	13	0.27
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	4	0.27
(1,422)	2:B:654:PHE:HB2	2:B:682:VAL:HG12	15	0.27
(1,422)	2:B:654:PHE:HB2	2:B:682:VAL:HG11	15	0.27
(1,422)	2:B:654:PHE:HB2	2:B:682:VAL:HG13	15	0.27
(1,375)	2:B:644:GLU:H	2:B:643:VAL:HB	2	0.27
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	5	0.27
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	5	0.27
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	5	0.27
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	2	0.27
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	2	0.27
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	2	0.27
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	2	0.27
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	2	0.27
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	2	0.27
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	4	0.27
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	4	0.27
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	4	0.27
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	4	0.27
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	4	0.27
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	4	0.27
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	15	0.27
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	15	0.27
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	15	0.27
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	15	0.27
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	15	0.27
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	15	0.27
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	14	0.27
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	14	0.27
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	14	0.27
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	14	0.27
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	14	0.27
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	11	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG22	15	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG21	15	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:619:ILE:HG23	15	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG22	15	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG21	15	0.27
(1,2380)	2:B:620:GLU:HB3	2:B:629:VAL:HG23	15	0.27
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	3	0.27
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	3	0.27
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	3	0.27
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	1	0.27
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	4	0.27
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	14	0.27
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	15	0.27
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	13	0.27
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	14	0.27
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	13	0.27
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	5	0.27
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	7	0.27
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD12	15	0.27
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD11	15	0.27
(1,1073)	2:B:579:SER:HB3	2:B:581:ILE:HD13	15	0.27
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	2	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	2	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	2	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	14	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	14	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	14	0.26
(1,854)	2:B:638:ARG:HG2	2:B:638:ARG:HD3	7	0.26
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD12	15	0.26
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD11	15	0.26
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD13	15	0.26
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	15	0.26
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	15	0.26
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	15	0.26
(1,54)	2:B:583:LEU:HD12	2:B:598:ASP:HB2	10	0.26
(1,54)	2:B:583:LEU:HD11	2:B:598:ASP:HB2	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	2:B:583:LEU:HD13	2:B:598:ASP:HB2	10	0.26
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	12	0.26
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	8	0.26
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	8	0.26
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	8	0.26
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	4	0.26
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	4	0.26
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	14	0.26
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	14	0.26
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	14	0.26
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	4	0.26
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	4	0.26
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	1	0.26
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	1	0.26
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	12	0.26
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	12	0.26
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	4	0.26
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	4	0.26
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	4	0.26
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	4	0.26
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	4	0.26
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	4	0.26
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	5	0.26
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	5	0.26
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	4	0.26
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	4	0.26
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	4	0.26
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	4	0.26
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	4	0.26
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	4	0.26
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	14	0.26
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	14	0.26
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	14	0.26
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	14	0.26
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	14	0.26
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	14	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	13	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	13	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	13	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	13	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	13	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	15	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	15	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	15	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	15	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	15	0.26
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	15	0.26
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	1	0.26
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	1	0.26
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	1	0.26
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	13	0.26
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	13	0.26
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	13	0.26
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	8	0.26
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	12	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	2	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	2	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	2	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG22	14	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG21	14	0.26
(1,2171)	2:B:683:CYS:H	2:B:682:VAL:HG23	14	0.26
(1,2132)	2:B:678:SER:H	2:B:678:SER:HB3	9	0.26
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	12	0.26
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	14	0.26
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	14	0.26
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	8	0.26
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	11	0.26
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	4	0.26
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	5	0.26
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	8	0.26
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	12	0.26
(1,1465)	2:B:580:ILE:H	2:B:579:SER:HB3	13	0.26
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	8	0.26
(1,1403)	1:A:41:VAL:HG22	1:A:39:SER:H	13	0.26
(1,1403)	1:A:41:VAL:HG21	1:A:39:SER:H	13	0.26
(1,1403)	1:A:41:VAL:HG23	1:A:39:SER:H	13	0.26
(1,1269)	2:B:672:LEU:HD22	2:B:575:PHE:HB2	5	0.26
(1,1269)	2:B:672:LEU:HD21	2:B:575:PHE:HB2	5	0.26
(1,1269)	2:B:672:LEU:HD23	2:B:575:PHE:HB2	5	0.26
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD22	15	0.26
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD21	15	0.26
(1,1216)	2:B:681:ASP:HB2	2:B:677:LEU:HD23	15	0.26
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	1	0.25
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	1	0.25
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	4	0.25
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	6	0.25
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	6	0.25
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	6	0.25
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	11	0.25
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	10	0.25
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	10	0.25
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	10	0.25
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	2	0.25
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	2	0.25
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	4	0.25
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	4	0.25
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	9	0.25
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	9	0.25
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD22	4	0.25
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD21	4	0.25
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD23	4	0.25
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD22	4	0.25
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD21	4	0.25
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD23	4	0.25
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD22	4	0.25
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD21	4	0.25
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD23	4	0.25
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	9	0.25
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	6	0.25
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	13	0.25
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	2	0.25
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	1	0.25
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	2	0.25
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	4	0.25
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	9	0.25
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	6	0.25
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	13	0.25
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	14	0.25
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	13	0.25
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	9	0.25
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	9	0.25
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	9	0.25
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	13	0.25
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	2:B:669:LEU:HD12	2:B:648:GLU:HB2	13	0.24
(1,999)	2:B:669:LEU:HD11	2:B:648:GLU:HB2	13	0.24
(1,999)	2:B:669:LEU:HD13	2:B:648:GLU:HB2	13	0.24
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	6	0.24
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	8	0.24
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	8	0.24
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	8	0.24
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	12	0.24
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	3	0.24
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	3	0.24
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	6	0.24
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	6	0.24
(1,2622)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	6	0.24
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	6	0.24
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	6	0.24
(1,2622)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	6	0.24
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	4	0.24
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	4	0.24
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	4	0.24
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	4	0.24
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	4	0.24
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	4	0.24
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	5	0.24
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	5	0.24
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	1	0.24
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	1	0.24
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	1	0.24
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD22	10	0.24
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD21	10	0.24
(1,2268)	2:B:643:VAL:HG22	1:A:44:LEU:HD23	10	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD22	10	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD21	10	0.24
(1,2268)	2:B:643:VAL:HG21	1:A:44:LEU:HD23	10	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD22	10	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD21	10	0.24
(1,2268)	2:B:643:VAL:HG23	1:A:44:LEU:HD23	10	0.24
(1,2029)	2:B:662:CYS:H	2:B:660:SER:HB2	9	0.24
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	5	0.24
(1,1979)	2:B:655:GLY:H	2:B:654:PHE:HA	2	0.24
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	4	0.24
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	4	0.24
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	6	0.24
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	8	0.24
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	10	0.24
(1,1628)	2:B:600:ILE:H	2:B:600:ILE:HG12	5	0.24
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	3	0.24
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	9	0.24
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	8	0.24
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	4	0.24
(1,1425)	2:B:571:LEU:H	2:B:571:LEU:HB2	9	0.24
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	1	0.24
(1,101)	2:B:672:LEU:HD12	2:B:591:VAL:HB	9	0.24
(1,101)	2:B:672:LEU:HD11	2:B:591:VAL:HB	9	0.24
(1,101)	2:B:672:LEU:HD13	2:B:591:VAL:HB	9	0.24
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	1	0.23
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	15	0.23
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	15	0.23
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	15	0.23
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	11	0.23
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	8	0.23
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	8	0.23
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	8	0.23
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	8	0.23
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	8	0.23
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	8	0.23
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	9	0.23
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	9	0.23
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	9	0.23
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	11	0.23
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	11	0.23
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	11	0.23
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	14	0.23
(1,2846)	2:B:649:TYR:H	2:B:575:PHE:HB2	10	0.23
(1,2846)	2:B:649:TYR:H	2:B:645:VAL:HB	10	0.23
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	1	0.23
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	1	0.23
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	1	0.23
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	1	0.23
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	1	0.23
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	1	0.23
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	1	0.23
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	1	0.23
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	1	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	10	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	10	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	10	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	10	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	10	0.23
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	10	0.23
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	12	0.23
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	12	0.23
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	12	0.23
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	12	0.23
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	12	0.23
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	12	0.23
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	12	0.23
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	12	0.23
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	12	0.23
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	10	0.23
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	13	0.23
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	1	0.23
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	15	0.23
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	12	0.23
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	13	0.23
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	13	0.23
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	6	0.23
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	11	0.23
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	3	0.23
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD22	3	0.23
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD21	3	0.23
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD23	3	0.23
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	10	0.23
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	11	0.22
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	11	0.22
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	11	0.22
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	9	0.22
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	4	0.22
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	4	0.22
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	4	0.22
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	4	0.22
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	4	0.22
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	4	0.22
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	15	0.22
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	15	0.22
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	15	0.22
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	15	0.22
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	15	0.22
(1,69)	2:B:587:GLU:HG3	2:B:587:GLU:HA	9	0.22
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	5	0.22
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	5	0.22
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	5	0.22
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	9	0.22
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	9	0.22
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	9	0.22
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	8	0.22
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	8	0.22
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	8	0.22
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	10	0.22
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	10	0.22
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	10	0.22
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	12	0.22
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	12	0.22
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	12	0.22
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	12	0.22
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	10	0.22
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	10	0.22
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	10	0.22
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	12	0.22
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	12	0.22
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	12	0.22
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	12	0.22
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	12	0.22
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	12	0.22
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	6	0.22
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	6	0.22
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	1	0.22
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	1	0.22
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	1	0.22
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	1	0.22
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	1	0.22
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	1	0.22
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	6	0.22
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	6	0.22
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	6	0.22
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	5	0.22
(1,211)	2:B:611:ILE:H	2:B:610:LYS:HB2	8	0.22
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	15	0.22
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	3	0.22
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	6	0.22
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	8	0.22
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	8	0.22
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	8	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	8	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	8	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	8	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG22	10	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG21	10	0.22
(1,1559)	2:B:592:GLU:H	2:B:591:VAL:HG23	10	0.22
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	3	0.22
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	11	0.22
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	11	0.22
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	11	0.22
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	8	0.22
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	9	0.22
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG21	6	0.22
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG22	6	0.22
(1,1057)	2:B:650:PRO:HG2	2:B:666:THR:HG23	6	0.22
(1,103)	2:B:672:LEU:HD12	2:B:672:LEU:HA	5	0.22
(1,103)	2:B:672:LEU:HD11	2:B:672:LEU:HA	5	0.22
(1,103)	2:B:672:LEU:HD13	2:B:672:LEU:HA	5	0.22
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	1	0.22
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	6	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	6	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	6	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	12	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	12	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	12	0.21
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	9	0.21
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	5	0.21
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	12	0.21
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	12	0.21
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	12	0.21
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	4	0.21
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	4	0.21
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	4	0.21
(1,510)	2:B:682:VAL:HG22	2:B:613:SER:HB2	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	2:B:682:VAL:HG21	2:B:613:SER:HB2	3	0.21
(1,510)	2:B:682:VAL:HG23	2:B:613:SER:HB2	3	0.21
(1,2962)	2:B:641:VAL:HG22	1:A:45:ALA:HA	15	0.21
(1,2962)	2:B:641:VAL:HG21	1:A:45:ALA:HA	15	0.21
(1,2962)	2:B:641:VAL:HG23	1:A:45:ALA:HA	15	0.21
(1,2962)	2:B:641:VAL:HG22	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:641:VAL:HG21	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:641:VAL:HG23	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:634:VAL:HG12	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:634:VAL:HG11	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:634:VAL:HG13	1:A:47:SER:HA	15	0.21
(1,2962)	2:B:645:VAL:HG22	1:A:44:LEU:HA	15	0.21
(1,2962)	2:B:645:VAL:HG21	1:A:44:LEU:HA	15	0.21
(1,2962)	2:B:645:VAL:HG23	1:A:44:LEU:HA	15	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	12	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	12	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	12	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	13	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	13	0.21
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	13	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	15	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	15	0.21
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	15	0.21
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	13	0.21
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	13	0.21
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	14	0.21
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	14	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG22	4	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG21	4	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG23	4	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG12	4	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG11	4	0.21
(1,2320)	2:B:617:GLU:HG3	2:B:679:VAL:HG13	4	0.21
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	10	0.21
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	10	0.21
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	10	0.21
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	8	0.21
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	8	0.21
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	8	0.21
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	8	0.21
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	8	0.21
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	8	0.21
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	8	0.21
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	8	0.21
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD12	7	0.21
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD11	7	0.21
(1,2267)	2:B:643:VAL:HG22	1:A:44:LEU:HD13	7	0.21
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD12	7	0.21
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD11	7	0.21
(1,2267)	2:B:643:VAL:HG21	1:A:44:LEU:HD13	7	0.21
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD12	7	0.21
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD11	7	0.21
(1,2267)	2:B:643:VAL:HG23	1:A:44:LEU:HD13	7	0.21
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	2	0.21
(1,2176)	2:B:684:ILE:H	2:B:684:ILE:HG12	15	0.21
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	6	0.21
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	7	0.21
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	7	0.21
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	10	0.21
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	14	0.21
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	10	0.21
(1,192)	2:B:585:ASN:HB3	2:B:605:ILE:HD12	9	0.21
(1,192)	2:B:585:ASN:HB3	2:B:605:ILE:HD11	9	0.21
(1,192)	2:B:585:ASN:HB3	2:B:605:ILE:HD13	9	0.21
(1,1782)	2:B:622:SER:H	2:B:621:ASP:HB2	13	0.21
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	15	0.21
(1,1533)	2:B:589:LYS:H	2:B:589:LYS:HB3	14	0.21
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	4	0.21
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	7	0.21
(1,1430)	2:B:575:PHE:H	2:B:576:MET:H	1	0.21
(1,1417)	1:A:44:LEU:HD12	1:A:45:ALA:H	8	0.21
(1,1417)	1:A:44:LEU:HD11	1:A:45:ALA:H	8	0.21
(1,1417)	1:A:44:LEU:HD13	1:A:45:ALA:H	8	0.21
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	7	0.21
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD22	15	0.21
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD21	15	0.21
(1,1219)	2:B:659:SER:HB2	2:B:677:LEU:HD23	15	0.21
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	2	0.21
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	3	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	3	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	3	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	4	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	4	0.2
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	1	0.2
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	7	0.2
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	14	0.2
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	14	0.2
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	14	0.2
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	14	0.2
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	14	0.2
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	14	0.2
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	7	0.2
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	7	0.2
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	7	0.2
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	15	0.2
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	15	0.2
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	15	0.2
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	3	0.2
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	1	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG22	15	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG21	15	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG23	15	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD12	15	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD11	15	0.2
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD13	15	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	5	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	5	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	5	0.2
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	5	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	9	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	9	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	9	0.2
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	9	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	15	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	15	0.2
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	15	0.2
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	15	0.2
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	6	0.2
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	6	0.2
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	7	0.2
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	7	0.2
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	7	0.2
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	15	0.2
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	15	0.2
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	15	0.2
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	15	0.2
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	15	0.2
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	9	0.2
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	1	0.2
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	7	0.2
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	11	0.2
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	8	0.2
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	7	0.2
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	10	0.2
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	6	0.2
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD12	14	0.2
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD11	14	0.2
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD13	14	0.2
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	14	0.2
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	7	0.19
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	7	0.19
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	7	0.19
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	13	0.19
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	13	0.19
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	13	0.19
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	11	0.19
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	11	0.19
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	11	0.19
(1,797)	2:B:660:SER:HB2	1:A:40:LEU:HA	6	0.19
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	9	0.19
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	9	0.19
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	9	0.19
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	9	0.19
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	9	0.19
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	9	0.19
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	1	0.19
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	2	0.19
(1,712)	2:B:603:ALA:HA	2:B:606:SER:HA	11	0.19
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD12	5	0.19
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD11	5	0.19
(1,697)	2:B:600:ILE:H	2:B:600:ILE:HD13	5	0.19
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD12	9	0.19
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD11	9	0.19
(1,64)	2:B:587:GLU:HB2	2:B:583:LEU:HD13	9	0.19
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	2:B:686:LEU:HD12	2:B:611:ILE:HA	4	0.19
(1,552)	2:B:686:LEU:HD11	2:B:611:ILE:HA	4	0.19
(1,552)	2:B:686:LEU:HD13	2:B:611:ILE:HA	4	0.19
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	3	0.19
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	3	0.19
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	3	0.19
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	9	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG22	3	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG21	3	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG23	3	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG12	3	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG11	3	0.19
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG13	3	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	6	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	6	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	6	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	14	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	14	0.19
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	14	0.19
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	13	0.19
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	13	0.19
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	13	0.19
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	13	0.19
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	8	0.19
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	8	0.19
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	8	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	9	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	9	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	9	0.19
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	9	0.19
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	9	0.19
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	9	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	15	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	15	0.19
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	15	0.19
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	15	0.19
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	15	0.19
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	15	0.19
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	9	0.19
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	9	0.19
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	9	0.19
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	9	0.19
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	9	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	4	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	4	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	4	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	8	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	8	0.19
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	8	0.19
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	11	0.19
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	11	0.19
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	11	0.19
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	12	0.19
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	12	0.19
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	12	0.19
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB2	13	0.19
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB3	13	0.19
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	3	0.19
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	3	0.19
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	3	0.19
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	12	0.19
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	12	0.19
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	12	0.19
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	6	0.19
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	9	0.19
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	14	0.19
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	8	0.19
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	14	0.19
(1,1891)	2:B:639:ALA:H	2:B:637:HIS:HB3	5	0.19
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	2	0.19
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	11	0.19
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	7	0.19
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	2	0.19
(1,1465)	2:B:580:ILE:H	2:B:579:SER:HB3	1	0.19
(1,1465)	2:B:580:ILE:H	2:B:579:SER:HB3	15	0.19
(1,1312)	2:B:654:PHE:HB3	2:B:684:ILE:HG12	12	0.19
(1,1086)	2:B:609:LEU:HD22	1:A:37:TRP:HZ3	7	0.19
(1,1086)	2:B:609:LEU:HD21	1:A:37:TRP:HZ3	7	0.19
(1,1086)	2:B:609:LEU:HD23	1:A:37:TRP:HZ3	7	0.19
(1,102)	2:B:672:LEU:HD12	2:B:673:PRO:HD3	8	0.19
(1,102)	2:B:672:LEU:HD11	2:B:673:PRO:HD3	8	0.19
(1,102)	2:B:672:LEU:HD13	2:B:673:PRO:HD3	8	0.19
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	12	0.19
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	3	0.18
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	6	0.18
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	7	0.18
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	4	0.18
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	4	0.18
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	4	0.18
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	10	0.18
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	10	0.18
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	10	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	7	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	7	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	7	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	7	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	7	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	7	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	10	0.18
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	10	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	10	0.18
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	10	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	10	0.18
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	10	0.18
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE2	4	0.18
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE3	4	0.18
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	10	0.18
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	4	0.18
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	4	0.18
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	4	0.18
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	4	0.18
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	4	0.18
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	4	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG22	14	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG21	14	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG23	14	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG12	14	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG11	14	0.18
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG13	14	0.18
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	15	0.18
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	15	0.18
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	15	0.18
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	3	0.18
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	3	0.18
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	3	0.18
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	3	0.18
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	3	0.18
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	13	0.18
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	13	0.18
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	13	0.18
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	15	0.18
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	15	0.18
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	15	0.18
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	15	0.18
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	15	0.18
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	15	0.18
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	7	0.18
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	7	0.18
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	7	0.18
(1,1980)	2:B:655:GLY:H	2:B:654:PHE:HB2	12	0.18
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	3	0.18
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	6	0.18
(1,1835)	2:B:627:VAL:H	2:B:646:LEU:HA	12	0.18
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	8	0.18
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	13	0.18
(1,1424)	2:B:571:LEU:H	2:B:570:THR:HA	2	0.18
(1,1298)	2:B:615:THR:HA	2:B:682:VAL:HB	2	0.18
(1,1298)	2:B:615:THR:HA	2:B:682:VAL:HB	9	0.18
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	1	0.18
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	1	0.18
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	1	0.18
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	1	0.18
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	2	0.18
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	2	0.18
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	10	0.17
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	11	0.17
(2,2)	2:B:595:LYS:HD2	2:B:658:TRP:HB3	4	0.17
(1,988)	2:B:647:VAL:HB	2:B:662:CYS:HB2	4	0.17
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	8	0.17
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	8	0.17
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	8	0.17
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	1	0.17
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	1	0.17
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	1	0.17
(1,911)	2:B:672:LEU:HD12	2:B:673:PRO:HD2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	2:B:672:LEU:HD11	2:B:673:PRO:HD2	7	0.17
(1,911)	2:B:672:LEU:HD13	2:B:673:PRO:HD2	7	0.17
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	1	0.17
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	1	0.17
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	1	0.17
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	1	0.17
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	1	0.17
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	1	0.17
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	3	0.17
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	5	0.17
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	5	0.17
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	5	0.17
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	12	0.17
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	12	0.17
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	12	0.17
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	6	0.17
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	7	0.17
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	15	0.17
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	7	0.17
(1,2962)	2:B:641:VAL:HG22	1:A:45:ALA:HA	2	0.17
(1,2962)	2:B:641:VAL:HG21	1:A:45:ALA:HA	2	0.17
(1,2962)	2:B:641:VAL:HG23	1:A:45:ALA:HA	2	0.17
(1,2962)	2:B:641:VAL:HG22	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:641:VAL:HG21	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:641:VAL:HG23	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:634:VAL:HG12	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:634:VAL:HG11	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:634:VAL:HG13	1:A:47:SER:HA	2	0.17
(1,2962)	2:B:645:VAL:HG22	1:A:44:LEU:HA	2	0.17
(1,2962)	2:B:645:VAL:HG21	1:A:44:LEU:HA	2	0.17
(1,2962)	2:B:645:VAL:HG23	1:A:44:LEU:HA	2	0.17
(1,2933)	2:B:583:LEU:HA	1:A:37:TRP:HB2	5	0.17
(1,2933)	2:B:583:LEU:HA	1:A:37:TRP:HB3	5	0.17
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	1	0.17
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	1	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	3	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	3	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	3	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	9	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	9	0.17
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	9	0.17
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	9	0.17
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	15	0.17
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	15	0.17
(1,2866)	2:B:661:CYS:H	2:B:674:CYS:HB2	1	0.17
(1,2866)	2:B:651:PHE:H	2:B:674:CYS:HB2	1	0.17
(1,2866)	2:B:661:CYS:H	2:B:674:CYS:HB2	11	0.17
(1,2866)	2:B:651:PHE:H	2:B:674:CYS:HB2	11	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	8	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	8	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	8	0.17
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	8	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	11	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	11	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	11	0.17
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	11	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	14	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	14	0.17
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	14	0.17
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	14	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HG22	1	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HG21	1	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HG23	1	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HD12	1	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HD11	1	0.17
(1,2596)	2:B:574:TYR:HB3	2:B:581:ILE:HD13	1	0.17
(1,2531)	2:B:613:SER:HB3	2:B:682:VAL:HG12	2	0.17
(1,2531)	2:B:613:SER:HB3	2:B:682:VAL:HG11	2	0.17
(1,2531)	2:B:613:SER:HB3	2:B:682:VAL:HG13	2	0.17
(1,2531)	2:B:642:SER:HB3	2:B:643:VAL:HG22	2	0.17
(1,2531)	2:B:642:SER:HB3	2:B:643:VAL:HG21	2	0.17
(1,2531)	2:B:642:SER:HB3	2:B:643:VAL:HG23	2	0.17
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	15	0.17
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	15	0.17
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	15	0.17
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	15	0.17
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	15	0.17
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	4	0.17
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	4	0.17
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	4	0.17
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	5	0.17
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	5	0.17
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	14	0.17
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	14	0.17
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	14	0.17
(1,2269)	2:B:629:VAL:HG22	1:A:44:LEU:HB2	10	0.17
(1,2269)	2:B:629:VAL:HG21	1:A:44:LEU:HB2	10	0.17
(1,2269)	2:B:629:VAL:HG23	1:A:44:LEU:HB2	10	0.17
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	11	0.17
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	2	0.17
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	2	0.17
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	5	0.17
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	10	0.17
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	15	0.17
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	6	0.17
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	6	0.17
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	6	0.17
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	3	0.17
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	10	0.17
(1,152)	2:B:595:LYS:HG2	2:B:658:TRP:HB3	10	0.17
(1,152)	2:B:595:LYS:HG3	2:B:658:TRP:HB3	10	0.17
(1,1240)	2:B:600:ILE:HG12	2:B:597:GLU:HA	8	0.17
(1,105)	2:B:672:LEU:HD22	2:B:591:VAL:HB	7	0.17
(1,105)	2:B:672:LEU:HD21	2:B:591:VAL:HB	7	0.17
(1,105)	2:B:672:LEU:HD23	2:B:591:VAL:HB	7	0.17
(1,101)	2:B:672:LEU:HD12	2:B:591:VAL:HB	8	0.17
(1,101)	2:B:672:LEU:HD11	2:B:591:VAL:HB	8	0.17
(1,101)	2:B:672:LEU:HD13	2:B:591:VAL:HB	8	0.17
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	10	0.17
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	13	0.17
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	15	0.17
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	5	0.16
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	8	0.16
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	10	0.16
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	5	0.16
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	5	0.16
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	5	0.16
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	5	0.16
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	5	0.16
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	5	0.16
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	11	0.16
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	11	0.16
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	11	0.16
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	11	0.16
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	11	0.16
(1,383)	2:B:646:LEU:H	2:B:645:VAL:HB	14	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:44:LEU:HG	6	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:44:LEU:HG	6	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:44:LEU:HG	6	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB2	6	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB1	6	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB3	6	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB2	6	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB1	6	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB3	6	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB2	6	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB1	6	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB3	6	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:44:LEU:HG	15	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:44:LEU:HG	15	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:44:LEU:HG	15	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB2	15	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB1	15	0.16
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB3	15	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB2	15	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB1	15	0.16
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB3	15	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB2	15	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB1	15	0.16
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB3	15	0.16
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	6	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	6	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	6	0.16
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	6	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	6	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	6	0.16
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	7	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	7	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	7	0.16
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	7	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	7	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	7	0.16
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	8	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	8	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	8	0.16
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	8	0.16
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	8	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	6	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	6	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	7	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	7	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	11	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	11	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	14	0.16
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	14	0.16
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	7	0.16
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	7	0.16
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	14	0.16
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	14	0.16
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	13	0.16
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	13	0.16
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	13	0.16
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	13	0.16
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	13	0.16
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	13	0.16
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	13	0.16
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	13	0.16
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	13	0.16
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	4	0.16
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	4	0.16
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	4	0.16
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	11	0.16
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	11	0.16
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	11	0.16
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	8	0.16
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	8	0.16
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	8	0.16
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	8	0.16
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	8	0.16
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	8	0.16
(1,2457)	2:B:674:CYS:HB3	2:B:666:THR:HA	4	0.16
(1,2457)	2:B:674:CYS:HB3	2:B:667:SER:HA	4	0.16
(1,2397)	2:B:629:VAL:HG22	2:B:617:GLU:HA	3	0.16
(1,2397)	2:B:629:VAL:HG21	2:B:617:GLU:HA	3	0.16
(1,2397)	2:B:629:VAL:HG23	2:B:617:GLU:HA	3	0.16
(1,2397)	2:B:629:VAL:HG22	2:B:641:VAL:HA	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2397)	2:B:629:VAL:HG21	2:B:641:VAL:HA	3	0.16
(1,2397)	2:B:629:VAL:HG23	2:B:641:VAL:HA	3	0.16
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	2	0.16
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	2	0.16
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	2	0.16
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	3	0.16
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	3	0.16
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	3	0.16
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	9	0.16
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	9	0.16
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	9	0.16
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	8	0.16
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	8	0.16
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	8	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	6	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	6	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	6	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	6	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	6	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	6	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	6	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	6	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	6	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD12	14	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD11	14	0.16
(1,2270)	2:B:641:VAL:HG12	1:A:44:LEU:HD13	14	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD12	14	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD11	14	0.16
(1,2270)	2:B:641:VAL:HG11	1:A:44:LEU:HD13	14	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD12	14	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD11	14	0.16
(1,2270)	2:B:641:VAL:HG13	1:A:44:LEU:HD13	14	0.16
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	15	0.16
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	15	0.16
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	15	0.16
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	12	0.16
(1,2001)	2:B:658:TRP:HE1	2:B:594:LEU:HB2	10	0.16
(1,198)	2:B:608:ASP:HB2	2:B:689:LYS:HB2	14	0.16
(1,198)	2:B:608:ASP:HB3	2:B:689:LYS:HB2	14	0.16
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	10	0.16
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	10	0.16
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	9	0.16
(1,1541)	2:B:590:LYS:H	2:B:589:LYS:HE2	13	0.16
(1,149)	2:B:596:THR:H	2:B:595:LYS:HB2	2	0.16
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	3	0.16
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	15	0.16
(1,1417)	1:A:44:LEU:HD12	1:A:45:ALA:H	10	0.16
(1,1417)	1:A:44:LEU:HD11	1:A:45:ALA:H	10	0.16
(1,1417)	1:A:44:LEU:HD13	1:A:45:ALA:H	10	0.16
(1,1298)	2:B:615:THR:HA	2:B:682:VAL:HB	1	0.16
(1,1298)	2:B:615:THR:HA	2:B:682:VAL:HB	5	0.16
(1,1240)	2:B:600:ILE:HG12	2:B:597:GLU:HA	2	0.16
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	9	0.16
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	9	0.16
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	4	0.15
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	9	0.15
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	9	0.15
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	9	0.15
(1,950)	2:B:572:PRO:HB2	2:B:573:PRO:HD3	15	0.15
(1,931)	2:B:639:ALA:HB2	2:B:634:VAL:HG22	4	0.15
(1,931)	2:B:639:ALA:HB2	2:B:634:VAL:HG21	4	0.15
(1,931)	2:B:639:ALA:HB2	2:B:634:VAL:HG23	4	0.15
(1,931)	2:B:639:ALA:HB1	2:B:634:VAL:HG22	4	0.15
(1,931)	2:B:639:ALA:HB1	2:B:634:VAL:HG21	4	0.15
(1,931)	2:B:639:ALA:HB1	2:B:634:VAL:HG23	4	0.15
(1,931)	2:B:639:ALA:HB3	2:B:634:VAL:HG22	4	0.15
(1,931)	2:B:639:ALA:HB3	2:B:634:VAL:HG21	4	0.15
(1,931)	2:B:639:ALA:HB3	2:B:634:VAL:HG23	4	0.15
(1,641)	2:B:683:CYS:HB3	2:B:651:PHE:HB2	1	0.15
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	14	0.15
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	14	0.15
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	14	0.15
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	2	0.15
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	3	0.15
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	3	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	3	0.15
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	3	0.15
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	3	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	3	0.15
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	9	0.15
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	9	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	9	0.15
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	9	0.15
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	9	0.15
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	11	0.15
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	11	0.15
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	4	0.15
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	4	0.15
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	4	0.15
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	8	0.15
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	8	0.15
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	8	0.15
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	10	0.15
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	10	0.15
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	10	0.15
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	10	0.15
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	10	0.15
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	10	0.15
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	6	0.15
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	6	0.15
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	6	0.15
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	6	0.15
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	6	0.15
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	6	0.15
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	2	0.15
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	2	0.15
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	7	0.15
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	7	0.15
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	8	0.15
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	8	0.15
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	10	0.15
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	10	0.15
(1,2499)	2:B:619:ILE:H	2:B:619:ILE:HG12	11	0.15
(1,2499)	2:B:679:VAL:H	2:B:619:ILE:HG12	11	0.15
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	3	0.15
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	3	0.15
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	3	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	3	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	3	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	3	0.15
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	3	0.15
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	3	0.15
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	3	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	10	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	10	0.15
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	10	0.15
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	10	0.15
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	10	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	12	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	12	0.15
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	12	0.15
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	12	0.15
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	12	0.15
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	12	0.15
(1,2397)	2:B:629:VAL:HG22	2:B:617:GLU:HA	11	0.15
(1,2397)	2:B:629:VAL:HG21	2:B:617:GLU:HA	11	0.15
(1,2397)	2:B:629:VAL:HG23	2:B:617:GLU:HA	11	0.15
(1,2397)	2:B:629:VAL:HG22	2:B:641:VAL:HA	11	0.15
(1,2397)	2:B:629:VAL:HG21	2:B:641:VAL:HA	11	0.15
(1,2397)	2:B:629:VAL:HG23	2:B:641:VAL:HA	11	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	3	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	3	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	3	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	3	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	3	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	3	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	8	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	8	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	8	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	8	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	8	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	8	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	12	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	12	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	12	0.15
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	12	0.15
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	12	0.15
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	12	0.15
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	13	0.15
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	13	0.15
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	13	0.15
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB2	2	0.15
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB3	2	0.15
(1,2218)	2:B:666:THR:HG21	1:A:39:SER:HG	5	0.15
(1,2218)	2:B:666:THR:HG22	1:A:39:SER:HG	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2218)	2:B:666:THR:HG23	1:A:39:SER:HG	5	0.15
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	1	0.15
(1,2210)	2:B:579:SER:HA	1:A:39:SER:HG	4	0.15
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	15	0.15
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	15	0.15
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	15	0.15
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	4	0.15
(1,1697)	2:B:610:LYS:H	2:B:610:LYS:HG2	12	0.15
(1,1465)	2:B:580:ILE:H	2:B:579:SER:HB3	2	0.15
(1,1449)	2:B:577:LYS:H	2:B:672:LEU:HB3	2	0.15
(1,1327)	1:A:48:GLN:HG2	1:A:48:GLN:H	1	0.15
(1,1327)	1:A:48:GLN:HG3	1:A:48:GLN:H	1	0.15
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	2	0.15
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	4	0.15
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	9	0.15
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	10	0.15
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	10	0.15
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	10	0.15
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	2	0.14
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	14	0.14
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	2	0.14
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	2	0.14
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	2	0.14
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	2	0.14
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	2	0.14
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	2	0.14
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	12	0.14
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	12	0.14
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	12	0.14
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	12	0.14
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	12	0.14
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	12	0.14
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	7	0.14
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE2	15	0.14
(1,615)	2:B:590:LYS:HB3	2:B:590:LYS:HE3	15	0.14
(1,578)	2:B:577:LYS:HD3	2:B:671:ASP:HB2	14	0.14
(1,576)	2:B:577:LYS:HD2	2:B:671:ASP:HB2	15	0.14
(1,566)	2:B:688:LEU:HD22	1:A:38:HIS:H	11	0.14
(1,566)	2:B:688:LEU:HD21	1:A:38:HIS:H	11	0.14
(1,566)	2:B:688:LEU:HD23	1:A:38:HIS:H	11	0.14
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	10	0.14
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	10	0.14
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG22	5	0.14
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG21	5	0.14
(1,425)	2:B:654:PHE:HB3	2:B:682:VAL:HG23	5	0.14
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	4	0.14
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	4	0.14
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	4	0.14
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	6	0.14
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	6	0.14
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	12	0.14
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	12	0.14
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	10	0.14
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	10	0.14
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	10	0.14
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	10	0.14
(1,27)	2:B:577:LYS:HE2	2:B:577:LYS:HG3	7	0.14
(1,27)	2:B:577:LYS:HE3	2:B:577:LYS:HG3	7	0.14
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	8	0.14
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	8	0.14
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	6	0.14
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	6	0.14
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	6	0.14
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	6	0.14
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	6	0.14
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	6	0.14
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	6	0.14
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	6	0.14
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	6	0.14
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	6	0.14
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	6	0.14
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	6	0.14
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	10	0.14
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	10	0.14
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	10	0.14
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	10	0.14
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	10	0.14
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	10	0.14
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	10	0.14
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	10	0.14
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	10	0.14
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	11	0.14
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	11	0.14
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB2	8	0.14
(1,2263)	2:B:614:SER:HB2	1:A:47:SER:HB3	8	0.14
(1,2208)	2:B:674:CYS:HB3	1:A:40:LEU:HB2	14	0.14
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	7	0.14
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	7	0.14
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	7	0.14
(1,2019)	2:B:660:SER:H	2:B:663:PRO:HB2	13	0.14
(1,1982)	2:B:655:GLY:H	2:B:596:THR:HG21	2	0.14
(1,1982)	2:B:655:GLY:H	2:B:596:THR:HG22	2	0.14
(1,1982)	2:B:655:GLY:H	2:B:596:THR:HG23	2	0.14
(1,1967)	2:B:653:VAL:H	1:A:41:VAL:HA	1	0.14
(1,1901)	2:B:640:GLN:H	2:B:640:GLN:HG2	9	0.14
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	14	0.14
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	5	0.14
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	12	0.14
(1,1544)	2:B:590:LYS:H	2:B:590:LYS:HG2	15	0.14
(1,1525)	2:B:588:LEU:H	2:B:587:GLU:HB3	10	0.14
(1,133)	2:B:591:VAL:HG22	2:B:579:SER:HB2	13	0.14
(1,133)	2:B:591:VAL:HG21	2:B:579:SER:HB2	13	0.14
(1,133)	2:B:591:VAL:HG23	2:B:579:SER:HB2	13	0.14
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	15	0.14
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	15	0.14
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	15	0.14
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	15	0.14
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	15	0.14
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	7	0.14
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	1	0.13
(1,85)	2:B:588:LEU:HD22	2:B:582:GLN:HB3	9	0.13
(1,85)	2:B:588:LEU:HD21	2:B:582:GLN:HB3	9	0.13
(1,85)	2:B:588:LEU:HD23	2:B:582:GLN:HB3	9	0.13
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	13	0.13
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	13	0.13
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	13	0.13
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	13	0.13
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	13	0.13
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	13	0.13
(1,62)	2:B:586:GLY:HA3	2:B:587:GLU:HG3	12	0.13
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	1	0.13
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	1	0.13
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	1	0.13
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD12	6	0.13
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD11	6	0.13
(1,404)	2:B:648:GLU:HG3	2:B:669:LEU:HD13	6	0.13
(1,391)	2:B:646:LEU:H	2:B:646:LEU:HD12	3	0.13
(1,391)	2:B:646:LEU:H	2:B:646:LEU:HD11	3	0.13
(1,391)	2:B:646:LEU:H	2:B:646:LEU:HD13	3	0.13
(1,2962)	2:B:641:VAL:HG22	1:A:45:ALA:HA	13	0.13
(1,2962)	2:B:641:VAL:HG21	1:A:45:ALA:HA	13	0.13
(1,2962)	2:B:641:VAL:HG23	1:A:45:ALA:HA	13	0.13
(1,2962)	2:B:641:VAL:HG22	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:641:VAL:HG21	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:641:VAL:HG23	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:634:VAL:HG12	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:634:VAL:HG11	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:634:VAL:HG13	1:A:47:SER:HA	13	0.13
(1,2962)	2:B:645:VAL:HG22	1:A:44:LEU:HA	13	0.13
(1,2962)	2:B:645:VAL:HG21	1:A:44:LEU:HA	13	0.13
(1,2962)	2:B:645:VAL:HG23	1:A:44:LEU:HA	13	0.13
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	11	0.13
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	11	0.13
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	11	0.13
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	11	0.13
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	11	0.13
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG22	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG21	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG23	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG12	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG11	11	0.13
(1,2924)	2:B:580:ILE:HB	1:A:34:VAL:HG13	11	0.13
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HG2	12	0.13
(1,2898)	2:B:675:SER:H	2:B:673:PRO:HB2	12	0.13
(1,2866)	2:B:661:CYS:H	2:B:674:CYS:HB2	15	0.13
(1,2866)	2:B:651:PHE:H	2:B:674:CYS:HB2	15	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG22	5	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG21	5	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HG23	5	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD12	5	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD11	5	0.13
(1,2767)	2:B:600:ILE:H	2:B:600:ILE:HD13	5	0.13
(1,2654)	2:B:683:CYS:HB3	2:B:656:GLN:HB3	13	0.13
(1,2654)	2:B:674:CYS:HB2	2:B:656:GLN:HB3	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2654)	2:B:674:CYS:HB2	2:B:676:LYS:HD3	13	0.13
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	5	0.13
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	5	0.13
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	5	0.13
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	5	0.13
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	5	0.13
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	5	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	7	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	7	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	7	0.13
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	7	0.13
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	7	0.13
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	7	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	11	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	11	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	11	0.13
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	11	0.13
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	11	0.13
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	11	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG22	13	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG21	13	0.13
(1,2489)	2:B:656:GLN:HB2	2:B:653:VAL:HG23	13	0.13
(1,2489)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	13	0.13
(1,2489)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	13	0.13
(1,2489)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	13	0.13
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	7	0.13
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	7	0.13
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	7	0.13
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	7	0.13
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	7	0.13
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	7	0.13
(1,22)	2:B:571:LEU:HD22	2:B:571:LEU:HA	2	0.13
(1,22)	2:B:571:LEU:HD21	2:B:571:LEU:HA	2	0.13
(1,22)	2:B:571:LEU:HD23	2:B:571:LEU:HA	2	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	11	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	11	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	11	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	13	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	13	0.13
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	13	0.13
(1,2029)	2:B:662:CYS:H	2:B:660:SER:HB2	12	0.13
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	11	0.13
(1,1931)	2:B:679:VAL:H	2:B:678:SER:HB2	4	0.13
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	10	0.13
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	12	0.13
(1,1638)	2:B:601:GLN:H	2:B:601:GLN:HG2	15	0.13
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	14	0.13
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	4	0.13
(1,1437)	2:B:576:MET:H	2:B:576:MET:HG3	14	0.13
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	3	0.13
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	3	0.13
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	3	0.13
(1,1240)	2:B:600:ILE:HG12	2:B:597:GLU:HA	10	0.13
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD12	7	0.13
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD11	7	0.13
(1,1222)	2:B:601:GLN:HG3	2:B:605:ILE:HD13	7	0.13
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG2	5	0.13
(1,1205)	2:B:569:PRO:HA	2:B:568:PRO:HG3	5	0.13
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	2	0.13
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	5	0.13
(2,7)	2:B:578:GLY:HA3	2:B:590:LYS:HG3	15	0.12
(2,6)	2:B:590:LYS:HD2	2:B:589:LYS:HA	4	0.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	12	0.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	12	0.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	12	0.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	12	0.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	12	0.12
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	12	0.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	12	0.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	12	0.12
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	12	0.12
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE1	6	0.12
(1,763)	2:B:611:ILE:HD12	2:B:652:PHE:HE2	6	0.12
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE1	6	0.12
(1,763)	2:B:611:ILE:HD11	2:B:652:PHE:HE2	6	0.12
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE1	6	0.12
(1,763)	2:B:611:ILE:HD13	2:B:652:PHE:HE2	6	0.12
(1,66)	2:B:587:GLU:HG2	2:B:587:GLU:HA	11	0.12
(1,642)	2:B:683:CYS:HB2	2:B:651:PHE:HB2	12	0.12
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	2	0.12
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	2	0.12
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	2	0.12
(1,441)	2:B:594:LEU:HG	2:B:589:LYS:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	2:B:594:LEU:HG	2:B:589:LYS:HA	5	0.12
(1,427)	2:B:654:PHE:HB2	2:B:656:GLN:HE22	3	0.12
(1,387)	2:B:646:LEU:HB3	2:B:646:LEU:HD12	3	0.12
(1,387)	2:B:646:LEU:HB3	2:B:646:LEU:HD11	3	0.12
(1,387)	2:B:646:LEU:HB3	2:B:646:LEU:HD13	3	0.12
(1,303)	2:B:627:VAL:HB	2:B:624:SER:HB3	7	0.12
(1,2956)	2:B:641:VAL:HG12	1:A:44:LEU:HG	4	0.12
(1,2956)	2:B:641:VAL:HG11	1:A:44:LEU:HG	4	0.12
(1,2956)	2:B:641:VAL:HG13	1:A:44:LEU:HG	4	0.12
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB2	4	0.12
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB1	4	0.12
(1,2956)	2:B:641:VAL:HG12	1:A:45:ALA:HB3	4	0.12
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB2	4	0.12
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB1	4	0.12
(1,2956)	2:B:641:VAL:HG11	1:A:45:ALA:HB3	4	0.12
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB2	4	0.12
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB1	4	0.12
(1,2956)	2:B:641:VAL:HG13	1:A:45:ALA:HB3	4	0.12
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	13	0.12
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	13	0.12
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	13	0.12
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	13	0.12
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	13	0.12
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	13	0.12
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB2	15	0.12
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB2	15	0.12
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB2	15	0.12
(1,2934)	2:B:583:LEU:HD22	1:A:37:TRP:HB3	15	0.12
(1,2934)	2:B:583:LEU:HD21	1:A:37:TRP:HB3	15	0.12
(1,2934)	2:B:583:LEU:HD23	1:A:37:TRP:HB3	15	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG22	8	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG21	8	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG23	8	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG12	8	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG11	8	0.12
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG13	8	0.12
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	11	0.12
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	11	0.12
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	11	0.12
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	1	0.12
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	1	0.12
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	10	0.12
(1,2860)	2:B:659:SER:H	2:B:662:CYS:HA	13	0.12
(1,2860)	2:B:659:SER:H	2:B:675:SER:HA	13	0.12
(1,2845)	2:B:648:GLU:H	2:B:648:GLU:HG3	11	0.12
(1,2845)	2:B:648:GLU:H	2:B:648:GLU:HB2	11	0.12
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG22	2	0.12
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG21	2	0.12
(1,2738)	2:B:593:ASP:H	2:B:591:VAL:HG23	2	0.12
(1,2738)	2:B:679:VAL:H	2:B:619:ILE:HG12	2	0.12
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	11	0.12
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	11	0.12
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	11	0.12
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	11	0.12
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	11	0.12
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	11	0.12
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HG3	13	0.12
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HG3	13	0.12
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HG3	13	0.12
(1,2351)	2:B:653:VAL:HG12	2:B:656:GLN:HB2	13	0.12
(1,2351)	2:B:653:VAL:HG11	2:B:656:GLN:HB2	13	0.12
(1,2351)	2:B:653:VAL:HG13	2:B:656:GLN:HB2	13	0.12
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	6	0.12
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	6	0.12
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	6	0.12
(1,2279)	2:B:581:ILE:HG22	1:A:37:TRP:HA	8	0.12
(1,2279)	2:B:581:ILE:HG21	1:A:37:TRP:HA	8	0.12
(1,2279)	2:B:581:ILE:HG23	1:A:37:TRP:HA	8	0.12
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	13	0.12
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	13	0.12
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	13	0.12
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	7	0.12
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	7	0.12
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	7	0.12
(1,2247)	2:B:609:LEU:HD12	1:A:37:TRP:HZ2	13	0.12
(1,2247)	2:B:609:LEU:HD11	1:A:37:TRP:HZ2	13	0.12
(1,2247)	2:B:609:LEU:HD13	1:A:37:TRP:HZ2	13	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	2	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	2	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	2	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	12	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	12	0.12
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:B:611:ILE:H	2:B:610:LYS:HB2	11	0.12
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	2	0.12
(1,2107)	2:B:674:CYS:H	2:B:674:CYS:HB3	8	0.12
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	1	0.12
(1,2018)	2:B:660:SER:H	2:B:674:CYS:HB2	9	0.12
(1,1953)	2:B:649:TYR:H	2:B:649:TYR:HB3	11	0.12
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	9	0.12
(1,1425)	2:B:571:LEU:H	2:B:571:LEU:HB2	1	0.12
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	8	0.12
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	8	0.12
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	8	0.12
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	8	0.12
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	14	0.12
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	14	0.12
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	14	0.12
(1,1211)	2:B:630:ILE:HA	2:B:619:ILE:HG13	7	0.12
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG22	6	0.11
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG21	6	0.11
(1,98)	2:B:672:LEU:HD12	2:B:591:VAL:HG23	6	0.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG22	6	0.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG21	6	0.11
(1,98)	2:B:672:LEU:HD11	2:B:591:VAL:HG23	6	0.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG22	6	0.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG21	6	0.11
(1,98)	2:B:672:LEU:HD13	2:B:591:VAL:HG23	6	0.11
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD22	10	0.11
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD21	10	0.11
(1,977)	2:B:574:TYR:HB2	1:A:40:LEU:HD23	10	0.11
(1,85)	2:B:588:LEU:HD22	2:B:582:GLN:HB3	2	0.11
(1,85)	2:B:588:LEU:HD21	2:B:582:GLN:HB3	2	0.11
(1,85)	2:B:588:LEU:HD23	2:B:582:GLN:HB3	2	0.11
(1,85)	2:B:588:LEU:HD22	2:B:582:GLN:HB3	5	0.11
(1,85)	2:B:588:LEU:HD21	2:B:582:GLN:HB3	5	0.11
(1,85)	2:B:588:LEU:HD23	2:B:582:GLN:HB3	5	0.11
(1,608)	2:B:589:LYS:HE2	2:B:589:LYS:HG3	3	0.11
(1,608)	2:B:589:LYS:HE2	2:B:589:LYS:HG3	4	0.11
(1,608)	2:B:589:LYS:HE2	2:B:589:LYS:HG3	9	0.11
(1,559)	2:B:688:LEU:H	2:B:688:LEU:HG	1	0.11
(1,534)	2:B:684:ILE:HG22	2:B:611:ILE:HB	13	0.11
(1,534)	2:B:684:ILE:HG21	2:B:611:ILE:HB	13	0.11
(1,534)	2:B:684:ILE:HG23	2:B:611:ILE:HB	13	0.11
(1,426)	2:B:654:PHE:HB3	2:B:656:GLN:HE22	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	2:B:653:VAL:HB	2:B:656:GLN:HB3	1	0.11
(1,2962)	2:B:641:VAL:HG22	1:A:45:ALA:HA	9	0.11
(1,2962)	2:B:641:VAL:HG21	1:A:45:ALA:HA	9	0.11
(1,2962)	2:B:641:VAL:HG23	1:A:45:ALA:HA	9	0.11
(1,2962)	2:B:641:VAL:HG22	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:641:VAL:HG21	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:641:VAL:HG23	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:634:VAL:HG12	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:634:VAL:HG11	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:634:VAL:HG13	1:A:47:SER:HA	9	0.11
(1,2962)	2:B:645:VAL:HG22	1:A:44:LEU:HA	9	0.11
(1,2962)	2:B:645:VAL:HG21	1:A:44:LEU:HA	9	0.11
(1,2962)	2:B:645:VAL:HG23	1:A:44:LEU:HA	9	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG22	8	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG21	8	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG23	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG22	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG21	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG23	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG22	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG21	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG23	8	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG12	8	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG11	8	0.11
(1,2953)	2:B:686:LEU:HD12	1:A:41:VAL:HG13	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG12	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG11	8	0.11
(1,2953)	2:B:686:LEU:HD11	1:A:41:VAL:HG13	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG12	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG11	8	0.11
(1,2953)	2:B:686:LEU:HD13	1:A:41:VAL:HG13	8	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG22	13	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG21	13	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG23	13	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG12	13	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG11	13	0.11
(1,2931)	2:B:582:GLN:HB2	1:A:34:VAL:HG13	13	0.11
(1,2930)	2:B:573:PRO:HB3	1:A:39:SER:HG	7	0.11
(1,2930)	2:B:576:MET:HB3	1:A:39:SER:HG	7	0.11
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG12	2	0.11
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG11	2	0.11
(1,291)	2:B:620:GLU:HB2	2:B:629:VAL:HG13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD12	7	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD11	7	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD13	7	0.11
(1,2643)	2:B:686:LEU:HD22	2:B:686:LEU:HA	7	0.11
(1,2643)	2:B:686:LEU:HD21	2:B:686:LEU:HA	7	0.11
(1,2643)	2:B:686:LEU:HD23	2:B:686:LEU:HA	7	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD12	15	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD11	15	0.11
(1,2643)	2:B:660:SER:HA	2:B:677:LEU:HD13	15	0.11
(1,2643)	2:B:686:LEU:HD22	2:B:686:LEU:HA	15	0.11
(1,2643)	2:B:686:LEU:HD21	2:B:686:LEU:HA	15	0.11
(1,2643)	2:B:686:LEU:HD23	2:B:686:LEU:HA	15	0.11
(1,2630)	2:B:673:PRO:HD3	2:B:577:LYS:HG2	13	0.11
(1,2630)	2:B:672:LEU:HB3	2:B:673:PRO:HD3	13	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	1	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	1	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	1	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	1	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	1	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	1	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	13	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	13	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	13	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	13	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	13	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	13	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:681:ASP:HB2	15	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:681:ASP:HB2	15	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:681:ASP:HB2	15	0.11
(1,2577)	2:B:630:ILE:HD12	2:B:683:CYS:HB3	15	0.11
(1,2577)	2:B:630:ILE:HD11	2:B:683:CYS:HB3	15	0.11
(1,2577)	2:B:630:ILE:HD13	2:B:683:CYS:HB3	15	0.11
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG21	10	0.11
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG22	10	0.11
(1,257)	2:B:617:GLU:HG3	2:B:615:THR:HG23	10	0.11
(1,2525)	2:B:611:ILE:HG22	1:A:37:TRP:HZ3	7	0.11
(1,2525)	2:B:611:ILE:HG21	1:A:37:TRP:HZ3	7	0.11
(1,2525)	2:B:611:ILE:HG23	1:A:37:TRP:HZ3	7	0.11
(1,2525)	2:B:611:ILE:HG22	2:B:599:PHE:H	7	0.11
(1,2525)	2:B:611:ILE:HG21	2:B:599:PHE:H	7	0.11
(1,2525)	2:B:611:ILE:HG23	2:B:599:PHE:H	7	0.11
(1,2490)	2:B:656:GLN:HB2	2:B:680:GLY:HA2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2490)	2:B:656:GLN:HB2	2:B:682:VAL:HA	10	0.11
(1,2490)	2:B:625:PRO:HB3	2:B:623:HIS:HA	10	0.11
(1,2478)	2:B:578:GLY:HA2	2:B:577:LYS:HB3	9	0.11
(1,2478)	2:B:590:LYS:HD3	2:B:578:GLY:HA2	9	0.11
(1,2317)	2:B:587:GLU:HB3	2:B:583:LEU:HB3	13	0.11
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HB3	13	0.11
(1,2317)	2:B:587:GLU:HB3	2:B:589:LYS:HG3	13	0.11
(1,2272)	2:B:641:VAL:HG12	1:A:44:LEU:HB3	9	0.11
(1,2272)	2:B:641:VAL:HG11	1:A:44:LEU:HB3	9	0.11
(1,2272)	2:B:641:VAL:HG13	1:A:44:LEU:HB3	9	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	1	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	1	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	1	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG12	4	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG11	4	0.11
(1,2144)	2:B:680:GLY:H	2:B:616:VAL:HG13	4	0.11
(1,211)	2:B:611:ILE:H	2:B:610:LYS:HB2	10	0.11
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG12	13	0.11
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG11	13	0.11
(1,1928)	2:B:645:VAL:H	2:B:645:VAL:HG13	13	0.11
(1,1901)	2:B:640:GLN:H	2:B:640:GLN:HG2	10	0.11
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	1	0.11
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	7	0.11
(1,1789)	2:B:624:SER:H	2:B:624:SER:HB3	13	0.11
(1,1570)	2:B:593:ASP:H	2:B:592:GLU:HG3	15	0.11
(1,1557)	2:B:592:GLU:H	2:B:590:LYS:HB2	13	0.11
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD22	9	0.11
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD21	9	0.11
(1,1427)	2:B:571:LEU:H	2:B:571:LEU:HD23	9	0.11
(1,1295)	2:B:589:LYS:HB2	2:B:590:LYS:H	5	0.11
(1,1288)	2:B:581:ILE:HG22	1:A:34:VAL:HA	2	0.11
(1,1288)	2:B:581:ILE:HG21	1:A:34:VAL:HA	2	0.11
(1,1288)	2:B:581:ILE:HG23	1:A:34:VAL:HA	2	0.11
(1,1240)	2:B:600:ILE:HG12	2:B:597:GLU:HA	9	0.11
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	6	0.11
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	8	0.11
(1,1090)	2:B:670:PHE:HB2	2:B:575:PHE:HZ	10	0.11
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	9	0.11
(1,1006)	2:B:652:PHE:HA	1:A:41:VAL:HA	11	0.11

10 Dihedral-angle violation analysis

No dihedral-angle restraints found